

Dortmund Data Bank (DDB)

Data for Pharmaceuticals

DDBST

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Introduction

The Dortmund Data Bank contains a variety of data for pharmaceuticals like solubilities, vapor-liquid equilibrium data and more. The purpose of this paper to to provide a statistics on available pharmaceuticals and amount of available related data.

For detailed information please contact DDBST (contact information is available on the title page).

Data Bank Content

The Dortmund Data Bank contains thermodynamic data for a variety of pure pharmaceuticals and of pharmaceuticals in mixtures with other components. The tables below give an overview on the amount of data separated by properties.

Summary

Databank	Description	Data Sets	Data Points	References
ACT	Activity Coefficients at Infinite Dilution	51	51	6
AZD	Azeotropy and Zeotropy	111	111	32
CPE	Excess Heat Capacities	22	179	4
CRI	Critical Data of Mixtures	2	22	1
ESLE	Salt Solubilities	19	87	5
GLE	Gas Solubilities	172	1136	22
HE	Heats of Mixing	39	705	7
LLE	Mixing Gaps (Liquid-liquid Equilibria)	89	344	14
PCP	Pure Component Properties (several properties)	615	1879	217
POW	Octanol-Water Partition Coefficients	312	312	56
SLE	Solid-liquid Equilibria (Solubilities)	1523	9642	190
VE	Densities, Volumes, Volume Effects of Mixing	86	705	18
VLE	Vapor-Liquid Equilibria (high-boiling components)	59	650	19
HPV	Vapor-Liquid Equilibria (low-boiling components)	437	3030	75
Total		3544	18991	(670)

Pure Component Properties

Property	Compounds	References	Data Sets	Data Points
Viscosity	9	11	14	50
Vapor Pressure	18	36	49	426
Critical Data	1	2	2	2
Triple Point	1	1	1	1
Density	15	31	38	156
Melting Point	100	121	272	411
Molar Heat Capacity (c_p)	12	12	15	404
Virial Coefficients	1	1	1	1
Heat of Vaporization	7	11	17	34
Heat of Fusion	47	47	100	102
Thermal Conductivity	1	1	1	2
Surface Tension	8	9	11	29
Std. Heat of Combustion	10	13	16	16
Std. Heat of Formation	12	18	21	21
Enthalpy (H-H0)	1	1	1	38
Enthalpy (H-H298)	1	1	2	29
G-function (G-G0)/T	1	1	1	8
Transition Temperature	24	9	31	31
Heat of Transition	5	6	11	11
Ideal Gas Heat Capacity	1	1	1	8
Dielectric Constant	3	3	7	39
Speed of Sound	1	1	2	22
Entropy (S-S0)	1	1	1	38
Total	115	217	615	1879

Components

DDB Code	Name	CAS Registry Number	Empirical Formula
18115	Sulfamic acid, lithium salt		H2LiNO3S
10018	1-Bromomethanesulfonamide	53412-78-5	CH4BrNO2S
319	2-Bromo-2-chloro-1,1,1-trifluoroethane	151-67-7	C2HBrClF3
1397	2,2-Dichloro-1,1-difluoro-1-methoxyethane	76-38-0	C3H4Cl2F2O
10020	1-Bromo-N,N-dimethylmethanesulfonamide	51270-39-4	C3H8BrNO2S
19396	Fluoroxene	406-90-6	C4H5F3O
3353	(D,L)-Tartaric acid	133-37-9	C4H6O6
3470	L-(+)-Tartaric acid	87-69-4	C4H6O6
6395	D-(-)-Tartaric acid	147-71-7	C4H6O6
10991	N-Amidinosarcosin	57-00-1	C4H9N3O2
3865	Piperazine	110-85-0	C4H10N2
12512	N,N-Dimethyl-ethanesulfonamide	6338-68-7	C4H11NO2S
10994	N-Amidinosarcosine hydrate	6020-87-7	C4H11N3O3
5223	1H-Purine-2,6-dione, 3,7-dihydro-	69-89-6	C5H4N4O2
5220	1H-Purin-6-amine	73-24-5	C5H5N5
5763	3-Pyridinesulfonamide	2922-45-4	C5H6N2O2S
19365	N-Acetyl-L-cysteine	616-91-1	C5H9NO3S
3994	Nicotinic acid	59-67-6	C6H5NO2
5393	Nicotinamide	98-92-0	C6H6N2O
7465	o-Chlorobenzenesulfonamide	98-64-6	C6H6ClNO2S
5921	Benzenesulfonamide	98-10-2	C6H7NO2S
5109	4-Hydroxyphenylsulfonamide	1576-43-8	C6H7NO3S
2979	Sulfanilamide	63-74-1	C6H8N2O2S
14175	Metanilamide	98-18-0	C6H8N2O2S
14176	Orthanilamide	3306-62-5	C6H8N2O2S
3063	L-Ascorbic acid	50-81-7	C6H8O6
7698	1,4-Dimethylpiperazine-2,5-dione	5076-82-4	C6H10N2O2
12513	N,N-Diethyl-ethanesulfonamide	33718-39-7	C6H15NO2S

DDB Code	Name	CAS Registry Number	Empirical Formula
740	2-Hydroxy benzoic acid	69-72-7	C7H6O3
3875	4-Hydroxy benzoic acid	99-96-7	C7H6O3
4700	2-Aminobenzoic acid	118-92-3	C7H7NO2
6165	Benzoic acid, 4-sulfamide	138-41-0	C7H7NO4S
10019	1-Bromo-N-phenylmethanesulfonamide	54114-59-9	C7H8BrNO2S
3077	3,7-Dihydro-3,7-dimethyl-1H-purine-2,6-dione	83-67-0	C7H8N4O2
3027	Theophylline	58-55-9	C7H8N4O2
5394	Aquarius	58-93-5	C7H8ClN3O4S2
15082	p-Toluenesulfonamide	70-55-3	C7H9NO2S
15084	o-Toluenesulfonamide	88-19-7	C7H9NO2S
9814	N-Methylbenzenesulfonamide	5183-78-8	C7H9NO2S
5398	4-Amino-N-(aminoiminomethyl)benzenesulfonamide	57-67-0	C7H10N4O2S
2940	Methyl p-hydroxybenzoate	99-76-3	C8H8O3
833	Acetanilide	103-84-4	C8H9NO
6440	4-Aminobenzoic acid methyl ester	619-45-4	C8H9NO2
6465	N-Acetyl-p-aminophenol	103-90-2	C8H9NO2
3079	3,7-Dihydro-1,3,7-trimethyl-1H-purine-2,6-dione	58-08-2	C8H10N4O2
16746	Sulfacetamide	144-80-9	C8H10N2O3S
3004	2-(3,4-Dihydroxyphenyl)-ethylamine	51-61-6	C8H11NO2
16647	N,N-Dimethyl benzenesulfonamide	14417-01-7	C8H11NO2S
15089	4-Ethylbenzene sulfamide	138-38-5	C8H11NO2S
15157	2,4-Dimethyl-benzenesulfonamide	7467-12-1	C8H11NO2S
15159	2,5-Dimethyl-benzenesulfonamide	6292-58-6	C8H11NO2S
15095	3-Ethyl benzene sulfamide		C8H11NO2S
15158	2,6-Dimethyl-benzenesulfonamide	24010-56-8	C8H11NO2S
3008	1-(3,4-Dihydroxyphenyl)-2-amino-ethanol	586-17-4	C8H11NO3
19394	Acyclovir	59277-89-3	C8H11N5O3
16423	Vitamin B6 hydrochloride	58-56-0	C8H12ClNO3
16409	6-APA	551-16-6	C8H12N2O3S
5806	6-Quinolinesulfonamide	89770-31-0	C9H8N2O2S

DDB Code	Name	CAS Registry Number	Empirical Formula
4776	2-Acetoxybenzoic acid <Acetylsalicylic acid>	50-78-2	C9H8O4
5872	2-[4'-Aminobenzensulfonamio]-thiazol	72-14-0	C9H9N3O2S2
504	Salicylic acid ethyl ester	118-61-6	C9H10O3
2941	Ethyl p-hydroxybenzoate	120-47-8	C9H10O3
6441	4-Aminobenzoic acid ethyl ester	94-09-7	C9H11NO2
5171	Preventol a 4	1085-98-9	C9H11Cl2FN2O2S2
18842	L-3,4-Dihydroxyphenylalanine	59-92-7	C9H11NO4
3003	3,4-Dihydroxy-DL-phenylalanine	63-84-3	C9H11NO4
16854	7-(2-Hydroxyethyl)theophylline	519-37-9	C9H12N4O3
5578	1-Propanesulfonamide, 3-(4-nitrophenoxy)-	105412-26-8	C9H12N2O5S
5697	Phenol, 4-(2-aminoethyl)-2-methoxy-	554-52-9	C9H13NO2
5692	m-Hydroxynorephedrine	54-49-9	C9H13NO2
3005	1-(4-Hydroxy-3-methoxyphenyl)-2-amino-ethanol	97-31-4	C9H13NO3
3006	DL-Adrenaline	329-65-7	C9H13NO3
5700	1,2-Benzenediol, 4-(2-amino-1-hydroxypropyl)-	6539-57-7	C9H13NO3
5699	DL-3-o-Methylnorepinephrine	709-52-4	C9H13NO3
20348	Scopoletin		C10H8O4
16456	Sulfadiazine	68-35-9	C10H10N4O2S
16747	Sulfamethoxazol	723-46-6	C10H11N3O3S
2510	Estragol <4-Methoxyallylbenzene>	140-67-0	C10H12O
6464	Propyl 4-hydroxybenzoate	94-13-3	C10H12O3
18204	Xanthosine	146-80-5	C10H12N4O6
6442	4-Aminobenzoic acid propyl ester	94-12-2	C10H13NO2
3864	Acetophenetidine	62-44-2	C10H13NO2
5022	(-)-Ephedrine <Ephedrine>	299-42-3	C10H15NO
3002	o-Methyladrenaline <Metanephrine>	5001-33-2	C10H15NO3
12676	2-Methyl-1,4-naphthochinone	58-27-5	C11H8O2
7509	N-3-Pyridinylbenzenesulfonamide	53472-19-8	C11H10N2O2S
16748	Sulfapyridine	144-83-2	C11H11N3O2S
776	Antipyrine	60-80-0	C11H12N2O

DDB Code	Name	CAS Registry Number	Empirical Formula
6085	N-(4-Methyl-2-pyrimidyl)sulfanilamide	127-79-7	C11H12N4O2S
5388	3-(p-Aminobenzenesulfamido)-6-methoxypyridazine	80-35-3	C11H12N4O3S
20278	Sulfisoxazole	127-69-5	C11H13N3O3S
5565	4-Hydroxybenzoic acid n-butyl ester	94-26-8	C11H14O3
6443	4-Aminobenzoic acid butyl ester	94-25-7	C11H15NO2
18214	(+)-N-Methylephedrine	42151-56-4	C11H17NO
18215	(+)-N-Methylephedrine	1201-56-5	C11H17NO
18213	(-)-N-Methylephedrine	552-79-4	C11H17NO
18925	1-(3,4-Dimethoxyphenyl)-2-propanamine	120-26-3	C11H17NO2
5694	Isoproterenol	7683-59-2	C11H17NO3
7512	N-(6-Methyl-2-pyridinyl) benzenesulfonamide	34456-75-2	C12H12N2O2S
5390	5-Ethyl-5-phenylbarbituric acid	50-06-6	C12H12N2O3
15108	2,7-Dimethyl 3-naphthalene sulfamide		C12H13NO2S
15103	3,7-Dimethyl 1-naphthalene sulfamide		C12H13NO2S
5387	N1-(4,6-Dimethyl-2-pyrimidinyl)-sulfanilamide	57-68-1	C12H14N4O2S
14016	Sulfanilic acid (2,6-dimethoxy-pyrimidine-4-ylamide)	122-11-2	C12H14N4O4S
18926	1-(2,3,4-Trimethoxyphenyl)-2-propanamine	22199-12-8	C12H19NO3
18921	1-(2,4,5-Trimethoxyphenyl)-2-propanamine	22199-15-1	C12H19NO3
18917	1-(3,4,5-Trimethoxyphenyl)-2-propanamine	22199-17-3	C12H19NO3
3001	3-Methoxyisoprenaline	1212-03-9	C12H19NO3
19563	Oxolinic acid	14698-29-4	C13H11NO5
17481	Nimesulide	51803-78-2	C13H12N2O5S
16385	(S)-(+)-Ibuprofen	51146-56-6	C13H18O2
5603	Ibuprofen	15687-27-1	C13H18O2
16384	(R)-(-)-Ibuprofen	51146-57-7	C13H18O2
3384	2-o-(a-D-Glucopyranosido)-benzyl alcohol	138-52-3	C13H18O7
5143	Nimrod	41483-43-6	C13H24N4O3S
17642	Khelline	82-02-0	C14H12O5
5439	Ally 20DF	74223-64-6	C14H15N5O6S
19404	rac-Boc-Piperazine		C14H27N3O3

DDB Code	Name	CAS Registry Number	Empirical Formula
19403	(S)-Boc-Piperazine	150323-35-6	C14H27N3O3
16666	Lorazepam	846-49-1	C15H10Cl2N2O2
18093	Quercetin	117-39-5	C15H10O7
20277	Nordazepam	1088-11-5	C15H11ClN2O
7520	n-(5-Bromo-8-quinolinyl)benzenesulfonamide	16082-63-6	C15H11BrN2O2S
12856	3-Hydroxynordiazepam	604-75-1	C15H11ClN2O2
7515	N-5-Quinolinylnbenzenesulfonamide	34298-61-8	C15H12N2O2S
7516	N-6-Quinolinylnbenzenesulfonamide	53472-22-3	C15H12N2O2S
7514	N-3-Quinolinylnbenzenesulfonamide	53472-21-2	C15H12N2O2S
7513	N-2-Quinolinylnbenzenesulfonamide	33757-75-4	C15H12N2O2S
20281	(-)-.alpha.-Santonin	481-06-1	C15H18O3
6084	Sulpiride	15676-16-1	C15H23N3O4S
15935	Diazepam	439-14-5	C16H13ClN2O
7517	N-(2-Methyl-4-quinolinyl)benzenesulfonamide	53472-23-4	C16H14N2O2S
7518	N-(2-Methyl-8-quinolinyl)benzenesulfonamide	15011-26-4	C16H14N2O2S
8460	Ketoprofen	22071-15-4	C16H14O3
19038	Valdecocixib	181695-72-7	C16H14N2O3S
7519	N-(6-Methoxy-8-quinolinyl)benzenesulfonamide	33757-70-9	C16H14N2O3S
13368	Benzylpenicillin potassium salt	113-98-4	C16H17KN2O4S
5724	Liquacillin	61-33-6	C16H18N2O4S
16406	6-[D-(-)-alpha-Amino-alpha-phenylacetamidol]-penicillanic acid	69-53-4	C16H19N3O4S
16407	6-[Amino-(4-hydroxyphenyl)-acetamido]-penicillan	26787-78-0	C16H19N3O5S
17321	Tetra-N-butylammonium sulfamate		C16H38N2O3S
5568	Triazolam	28911-01-5	C17H12Cl2N4
17640	Griseofulvin	126-07-8	C17H17ClO6
5771	Phenethicillin	147-55-7	C17H20N2O5S
5735	Penicillin, (2,6-dimethoxyphenyl)-	61-32-5	C17H20N2O6S
16452	Vitamine B2	83-88-5	C17H20N4O6
6714	Atropine	51-55-8	C17H23NO3

DDB Code	Name	CAS Registry Number	Empirical Formula
5125	Leponex (clozapin)	5786-21-0	C18H19ClN4
5488	4,4'-(1,2-Diethyl-1,2-ethenediyl)bisphenol	56-53-1	C18H20O2
6295	(RS)-Nitrendipine	39562-70-4	C18H20N2O6
20428	(R)-Nitrendipine		C18H20N2O6
20429	(S)-Nitrendipine		C18H20N2O6
18686	Estrone	53-16-7	C18H22O2
5722	Propicillin	551-27-9	C18H22N2O5S
14421	1,3,5-Oestratrien-3,17-beta-diol	50-28-2	C18H24O2
18685	Estriol	50-27-1	C18H24O3
5718	Dicloxacillin	3116-76-5	C19H17Cl2N3O5S
5719	Flucloxacillin	5250-39-5	C19H17ClFN3O5S
5720	Cloxacillin	61-72-3	C19H18ClN3O5S
5721	Prostaphlyn	66-79-5	C19H19N3O5S
18448	Phenylbutazone	50-33-9	C19H20N2O2
20244	Paroxetine hydrochloride		C19H21ClFNO3
3025	Testosterone	58-22-0	C19H28O2
18044	17-Ethinyl-1,3,5-extratriene-3,17-diol	57-63-6	C20H24O2
5347	Quinine	130-95-0	C20H24N2O2
5120	(9S)-6'-Methoxycinchonan-9-ol	56-54-2	C20H24N2O2
18682	Testosterone formate		C20H28O3
14968	All-trans-retinol	68-26-8	C20H30O
5566	Masenone	58-18-4	C20H30O2
5563	(-)-Prostaglandin E2 <PGE2>	363-24-6	C20H32O5
5564	Dinoprost	551-11-1	C20H34O5
18673	1-Cortisone	53-03-2	C21H26O5
18670	17-.alpha.-Ethinyltestosterone	434-03-7	C21H28O2
20211	16-alpha,17-alpha-Epoxyprogesterone		C21H28O3
19367	11-alpha-Hydroxy-16-alpha,17-alpha-epoxyprogesterone		C21H28O4
3024	Cortisone	53-06-5	C21H28O5

DDB Code	Name	CAS Registry Number	Empirical Formula
3026	Progesterone	57-83-0	C21H30O2
18681	Testosterone acetate	1045-69-8	C21H30O3
16739	11a-Hydroxy-4-pregnene-3,20-dione	80-75-1	C21H30O3
5017	Cortisol	50-23-7	C21H30O5
18663	Norethindrone acetate	51-98-9	C22H28O3
5982	Retinol acetate	127-47-9	C22H32O2
18665	Methyltestosterone acetate		C22H32O3
18671	Testosterone propionate	57-85-2	C22H32O3
20280	Quinine ethylcarbonate	83-75-0	C23H28N2O4
16725	Cortisone acetate	50-04-4	C23H30O6
15679	21-Acetoxy-4-pregnene-11,beta,17,alpha-diol-3,20-dione	50-03-3	C23H32O6
18683	Testosterone butyrate		C23H34O3
19047	Medroxyprogesterone acetate		C24H34O4
20279	Dehydrocholic acid	81-23-2	C24H34O5
18684	Testosterone valerate		C24H36O3
18669	17-.beta.-Estradiol-3-benzoate		C25H28O3
18664	Norethindrone enanthate		C27H38O3
14965	5,7-Cholestadien-3beta-ol	67-97-0	C27H44O
6456	Cholest-5-en-3-ol	57-88-5	C27H46O
18139	Provitamin D2	57-87-4	C28H44O
14966	Ergocalciferol	50-14-6	C28H44O
18986	Eflucimibe	202340-45-2	C29H43NO2S
18138	Stigmasterol	83-48-7	C29H48O
12713	2-(3,4Dimethoxyphenyl)-ethyl-(3-4-(2-isopropylindolizine-1-sulfonyl)-phenoxypropylmethylamin	114432-13-2	C31H38N2O5S
14967	2-Methyl-3-phythyl-1,4-naphthochinon	84-80-0	C31H46O2
5020	Atropine sulfate	55-48-1	C34H48N2O10S
20081	Ergocalciferol, 3,5-dinitribenzoate		C35H46N2O6
5981	Retinol palmitate	79-81-2	C36H60O2
3345	All-trans-beta-carotene	7235-40-7	C40H56

DDB Code	Name	CAS Registry Number	Empirical Formula
19677	Digoxin		C ₄₁ H ₆₄ O ₁₄