Dapsone

Other names:

1,1'-Sulfonylbis[4-aminobenzene]
1,1'-Sulphonylbis(4-aminobenzene)
1358F
4,4'-DDS
4,4'-Dapsone
4,4'-Diaminodiphenyl Sulfone
4,4'-Diaminodiphenyl sulphone
4,4'-Sulfonylbis[benzamine]
4,4'-Sulfonylbisaniline
4,4'-Sulfonylbisbenzeneamine
4,4'-Sulfonyldianiline
4,4'-Sulfonyldiphenylamine
4,4'-Sulphonylbisbenzamine
4,4'-Sulphonylbisbenzenamine
4,4'-Sulphonyldianiline
4,4'-sulfonylbisbenzamine
4,4'-sulfonylbisbenzenamine
4,4-Diaminodifenylsulfon
4-Aminophenyl sulfone
Aniline, 4,4'-sulfonyldi-
Araldite HT 976
Avlosulfon
Avlosulfone
Avlosulphone
Benzenamine, 4,4'-sulfonylbis-
Bis(4-aminophenyl) sulfone
Bis(4-aminophenyl)sulphone
Bis(p-aminophenyl) sulfone
Bis(p-aminophenyl)sulphone
Croysulfone
Croysulphone
DADPS
DDS
DDS, diaphenylsulfone
DDS, pharmaceutical
DSS
Dapson
Dapsonum
Di(4-aminophenyl) sulfone
Di(4-aminophenyl)sulphone

Di(p-aminophenyl) sulfone
Di(p-aminophenyl)sulphone
Diamino-4,4'-diphenyl sulfone
Diamino-4,4'-diphenyl sulphone
Diaminodifenilsulfona
Diaminodiphenyl sulfone
Dianiline, 4,4'-sulfonyl-
Diaphenyl sulfone
Diaphenylsulfon
Diaphenylsulphon
Diaphenylsulphone
Dimitone
Diphenasone
Diphone
Disulone
Dubronax
Dumitone
Eporal
F 1358
HT 9664
HT 976
ICI
Metabolite C
N,N'-Diphenyl sulfondiamide
NCI-C01718
NSC 6091D
NSC-6091
Novophone
Servidapson
Sulfadione
Sulfanona-mae
Sulfon-mere
Sulfona
Sulfona-MAE
Sulfone UCB
Sulfonyldianiline
Sulphadione
Sulphon-Mere
Sulphonyldianiline
Sumicure S
Tarimyl
Udolac
WR 448

	diaphenylsulfone
	p,p'-diaminodiphenyl sulfone
	p,p'-sulfonyldianiline
	p,p-Diaminodiphenyl sulphone
	p,p-Sulfonylbisbenzamine
	p,p-Sulfonylbisbenzenamine
	p,p-Sulphonylbisbenzamine
	p,p-Sulphonylbisbenzenamine
	p,p-Sulphonyldianiline
	p-Aminophenyl sulfone
	sulfone, 4-aminophenyl-
Inchi:	InChI=1S/C12H12N2O2S/c13-9-1-5-11(6-2-9)17(15,16)12-7-3-10(14)4-8-12/h1-8H,13-14
InchiKey:	MQJKPEGWNLWLTK-UHFFFAOYSA-N
Formula:	C12H12N2O2S
SMILES:	Nc1ccc(S(=O)(=O)c2ccc(N)cc2)cc1
Mol. weight [g/mol]:	248.30
CAS:	80-08-0

Physical Properties

Property code	Value	Unit	Source
gf	-79.92	kJ/mol	Joback Method
hf	-226.66	kJ/mol	Joback Method
hfus	35.91	kJ/mol	Joback Method
hvap	88.10	kJ/mol	Joback Method
ie	7.25	eV	NIST Webbook
ie	7.25 ± 0.05	eV	NIST Webbook
log10ws	-3.09		Estimated Solubility Method
log10ws	-2.93		Aqueous Solubility Prediction Method
log10ws	-3.09		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	1.684		Crippen Method
mcvol	180.470	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
rinpol	2880.00		NIST Webbook
tb	730.12	K	Joback Method
tc	981.90	K	Joback Method
tf	449.03	K	Aqueous Solubility Prediction Method

tf	451.00	K	NIST Webbook
tf	451.00 ± 1.00	K	NIST Webbook
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.17	J/mol×K	730.12	Joback Method
cpg	487.20	J/mol×K	772.08	Joback Method
cpg	498.94	J/mol×K	814.05	Joback Method
cpg	509.42	J/mol×K	856.01	Joback Method
cpg	518.70	J/mol×K	897.97	Joback Method
cpg	526.81	J/mol×K	939.93	Joback Method
cpg	533.79	J/mol×K	981.90	Joback Method
cps	314.90	J/mol×K	298.00	NIST Webbook

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80080&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Equilibrium solubility and preferential solvation of 1,1'-sulfonylbis(4-aminobenzene) in binary aqueous solutions of n-propanol, isopropanol and 1,4-dioxane:	https://www.doi.org/10.1016/j.jct.2018.03.010
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume