

3,5-Dichlorosulfanilamide

Other names:	Benzenesulfonamide, 4-amino-3,5-dichloro-Sulfanilamide, 3,5-dichloro-3,5-dichlorosulphanilamide
Inchi:	InChI=1S/C6H6Cl2N2O2S/c7-4-1-3(13(10,11)12)2-5(8)6(4)9/h1-2H,9H2,(H2,10,11,12)
InchiKey:	DVZMRTJKNJKEGV-UHFFFAOYSA-N
Formula:	C6H6Cl2N2O2S
SMILES:	<chem>Nc1c(Cl)cc(S(N)(=O)=O)cc1Cl</chem>
Mol. weight [g/mol]:	241.09
CAS:	22134-75-4

Physical Properties

Property code	Value	Unit	Source
gf	-276.34	kJ/mol	Joback Method
hf	-382.30	kJ/mol	Joback Method
hfus	34.34	kJ/mol	Joback Method
hvap	81.90	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.223		Crippen Method
mcvol	144.170	ml/mol	McGowan Method
pc	5800.57	kPa	Joback Method
tb	646.00	K	Joback Method
tc	887.94	K	Joback Method
tf	486.28	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.75	J/molxK	646.00	Joback Method
cpg	317.29	J/molxK	686.32	Joback Method
cpg	325.12	J/molxK	726.65	Joback Method
cpg	332.22	J/molxK	766.97	Joback Method
cpg	338.60	J/molxK	807.29	Joback Method
cpg	344.25	J/molxK	847.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22134754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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