

Benzothiazole, 2,6-dichloro-

Other names:	2,6-dichlorobenzothiazole
Inchi:	InChI=1S/C7H3Cl2NS/c8-4-1-2-5-6(3-4)11-7(9)10-5/h1-3H
InchiKey:	QDZGJGWDGLHVNK-UHFFFAOYSA-N
Formula:	C7H3Cl2NS
SMILES:	Clc1ccc2nc(Cl)sc2c1
Mol. weight [g/mol]:	204.08
CAS:	3622-23-9

Physical Properties

Property code	Value	Unit	Source
chs	-3895.90 ± 4.60	kJ/mol	NIST Webbook
hfs	62.80 ± 4.60	kJ/mol	NIST Webbook
log10ws	-4.17		Crippen Method
logp	3.603		Crippen Method
mcvol	121.380	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3622239&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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