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