2,6-Dichlorophenyl isothiocyanate

Inchi: InChI=1S/C7H3Cl2NS/c8-5-2-1-3-6(9)7(5)10-4-11/h1-3H
InchiKey: SUCGVQHNGIQXGD-UHFFFAOYSA-N
Formula: C7H3Cl2NS
SMILES: S=C=Nc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 204.08
CAS: 6590-95-0

Physical Properties

Property code	Value	Unit	Source
hf	278.37	kJ/mol	Joback Method
hvap	53.99	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.728		Crippen Method
mcvol	127.940	ml/mol	McGowan Method
pc	3713.49	kPa	Joback Method
tb	617.01	K	Joback Method
tc	892.29	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6590950&Units=SI

Legend

hf: Enthalpy of formation 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