2,4-Dichlorophenyl isothiocyanate

Other names: Benzene, 2,4-dichloro-1-isothiocyanato-
2,4-dichloro-1-isothiocyanatobenzene
Inchi: InChI=1S/C7H3Cl2NS/c8-5-1-2-7(10-4-11)6(9)3-5/h1-3H
InchiKey: WVBNZZHGECFCSH-UHFFFAOYSA-N
Formula: C7H3Cl2NS
SMILES: S=C=Nc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 204.08
CAS: 6590-96-1

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6590961&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

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