Benzene, 1-chloro-2-isothiocyanato-4-nitro-

Other names: 1-chloro-2-isothiocyanato-4-nitrobenzene
Inchi: InChI=1S/C7H3ClN2O2S/c8-6-2-1-5(10(11)12)3-7(6)9-4-13/h1-3H
InchiKey: QSSZYQDXSYYXKK-UHFFFAOYSA-N
Formula: C7H3ClN2O2S
SMILES: O=[N+]([O-])c1ccc(Cl)c(N=C=S)c1
Mol. weight [g/mol]: 214.63
CAS: 57135-68-9

Physical Properties

Property code	Value	Unit	Source
hf	283.35	kJ/mol	Joback Method
hvap	66.19	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.982		Crippen Method
mcvol	133.120	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
tb	731.42	K	Joback Method
tc	1024.55	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=C57135689&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