2-Chloro-5-trifluoromethylphenyl isothiocyanate

Inchi: InChI=1S/C8H3ClF3NS/c9-6-2-1-5(8(10,11)12)3-7(6)13-4-14/h1-3H
InchiKey: KHTMKXDMVYHDSY-UHFFFAOYSA-N
Formula: C8H3ClF3NS
SMILES: FC(F)(F)c1ccc(Cl)c(N=C=S)c1
Mol. weight [g/mol]: 237.63
CAS: 23165-49-3

Physical Properties

Property code	Value	Unit	Source
hf	-323.61	kJ/mol	Joback Method
hvap	48.08	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.093		Crippen Method
mcvol	135.100	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
tb	597.04	K	Joback Method
tc	839.12	K	Joback Method

Sources

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=C23165493&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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