

4-Chloro-3-trifluoromethylphenyl isothiocyanate

Inchi: InChI=1S/C8H3ClF3NS/c9-7-2-1-5(13-4-14)3-6(7)8(10,11)12/h1-3H
InchiKey: AHFPRSSHNSGRUC-UHFFFAOYSA-N
Formula: C8H3ClF3NS
SMILES: FC(F)(F)c1cc(N=C=S)ccc1Cl
Mol. weight [g/mol]: 237.63
CAS: 23163-86-2

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C23163862&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

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