3-Chloro-4-fluorophenyl isothiocyanate

Inchi: InChI=1S/C7H3ClFNS/c8-6-3-5(10-4-11)1-2-7(6)9/h1-3H
InchiKey: BUVRIIKIGKFOKD-UHFFFAOYSA-N
Formula: C7H3ClFNS
SMILES: Fc1ccc(N=C=S)cc1Cl
Mol. weight [g/mol]: 187.62
CAS: 137724-66-4

Physical Properties

Property code	Value	Unit	Source
hf	98.00	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.213		Crippen Method
mcvol	117.470	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method
tb	578.85	K	Joback Method
tc	836.59	K	Joback Method

Sources

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=C137724664&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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