Pentafluorophenyl isothiocyanate

Other names: Benzene, pentafluoroisothiocyanato-
perfluorophenyl isothiocyanate
Inchi: InChI=1S/C7F5NS/c8-2-3(9)5(11)7(13-1-14)6(12)4(2)10
InchiKey: NGNKMRBGZPDABE-UHFFFAOYSA-N
Formula: C7F5NS
SMILES: Fc1c(F)c(F)c(N=C=S)c(F)c1F
Mol. weight [g/mol]: 225.14
CAS: 35923-79-6

Physical Properties

Property code	Value	Unit	Source
hf	-705.11	kJ/mol	Joback Method
hvap	43.12	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.116		Crippen Method
mcvol	112.310	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
tb	553.44	K	Joback Method
tc	762.23	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35923796&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