2-Fluorophenyl isothiocyanate

Other names: o-Fluorophenyl isothiocyanate
Benzene, 1-fluoro-2-isothiocyanato-
Inchi: InChI=1S/C7H4FNS/c8-6-3-1-2-4-7(6)9-5-10/h1-4H
InchiKey: OAGDRIUTLPDSMJ-UHFFFAOYSA-N
Formula: C7H4FNS
SMILES: Fc1ccccc1N=C=S
Mol. weight [g/mol]: 153.18
CAS: 38985-64-7

Physical Properties

Property code	Value	Unit	Source
hf	125.21	kJ/mol	Joback Method
hvap	43.74	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.560		Crippen Method
mcvol	105.230	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
tb	339.00	K	NIST Webbook
tc	788.99	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=C38985647&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