Benzene, 1-fluoro-4-isothiocyanato-

Other names:	p-Fluorophenyl isothiocyanate
	4-Fluorophenyl isothiocyanate
	Isothiocyanic acid, p-fluorophenyl ester
Inchi:	InChI=1S/C7H4FNS/c8-6-1-3-7(4-2-6)9-5-10/h1-4H
InchiKey:	NFIUJHJMCQQYDL-UHFFFAOYSA-N
Formula:	C7H4FNS
SMILES:	Fc1ccc(N=C=S)cc1
Mol. weight [g/mol]:	153.18
CAS:	1544-68-9

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	536.44	K	Joback Method
tc	788.99	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1544689&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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