

5-Fluoro-2-methylphenyl isothiocyanate

Inchi: InChI=1S/C8H6FNS/c1-6-2-3-7(9)4-8(6)10-5-11/h2-4H,1H3
InchiKey: QVCYTKXGZLOVFA-UHFFFAOYSA-N
Formula: C8H6FNS
SMILES: Cc1ccc(F)cc1N=C=S
Mol. weight [g/mol]: 167.20
CAS: 175205-39-7

Physical Properties

Property code	Value	Unit	Source
hf	93.10	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.868		Crippen Method
mcvol	119.320	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	564.30	K	Joback Method
tc	812.59	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C175205397&Units=SI>
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>

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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