

2,3,5,6-Tetrafluorophenyl isothiocyanate

Inchi:	InChI=1S/C7HF4NS/c8-3-1-4(9)6(11)7(5(3)10)12-2-13/h1H
InchiKey:	QUNNLKBODYSOQL-UHFFFAOYSA-N
Formula:	C7HF4NS
SMILES:	Fc1cc(F)c(F)c(N=C=S)c1F
Mol. weight [g/mol]:	207.15
CAS:	20925-31-9

Physical Properties

Property code	Value	Unit	Source
hf	-497.53	kJ/mol	Joback Method
hvap	43.27	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.977		Crippen Method
mcvol	110.540	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	549.19	K	Joback Method
tc	767.64	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20925319&Units=SI

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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