2,5-Difluorophenyl isothiocyanate

Inchi: InChI=1S/C7H3F2NS/c8-5-1-2-6(9)7(3-5)10-4-11/h1-3H
InchiKey: QVIDXDRFMDPVLA-UHFFFAOYSA-N
Formula: C7H3F2NS
SMILES: Fc1ccc(F)c(N=C=S)c1
Mol. weight [g/mol]: 171.17
CAS: 206559-57-1

Physical Properties

Property code	Value	Unit	Source
hf	-82.37	kJ/mol	Joback Method
hvap	43.58	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.699		Crippen Method
mcvol	107.000	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	540.69	K	Joback Method
tc	780.96	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C206559571&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