2,6-Difluorophenyl isocyanate

Other names: 2,6-Difluorophenyl isothiocyanate
Inchi: InChI=1S/C7H3F2NS/c8-5-2-1-3-6(9)7(5)10-4-11/h1-3H
InchiKey: DBSXNGIBAKYMSS-UHFFFAOYSA-N
Formula: C7H3F2NO
SMILES: Fc1cccc(F)c1N=C=S
Mol. weight [g/mol]: 155.10
CAS: 65295-69-4

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

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=C65295694&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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