2-Fluoro-5-nitrophenyl isocyanate

Inchi: InChI=1S/C7H3FN2O3/c8-6-2-1-5(10(12)13)3-7(6)9-4-11/h1-3H
InchiKey: XCDYDLFUPMSLGZ-UHFFFAOYSA-N
Formula: C7H3FN2O3
SMILES: O=C=Nc1cc([N+](=O)[O-])ccc1F
Mol. weight [g/mol]: 182.11
CAS: 68622-14-0

Physical Properties

Property code	Value	Unit	Source
hf	-186.50	kJ/mol	Joback Method
hvap	60.08	kJ/mol	Joback Method
log10ws	-6.94		Crippen Method
logp	1.701		Crippen Method
mcvol	112.170	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
tb	613.98	K	Joback Method
tc	857.74	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=C68622140&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