4-Fluoro-3-nitrophenyl isocyanate

Other names: 4-Fluoro-5-nitrophenyl isocyanate
Inchi: InChI=1S/C7H3FN2O3/c8-6-2-1-5(9-4-11)3-7(6)10(12)13/h1-3H
InchiKey: KCHOHFPMTUPOJU-UHFFFAOYSA-N
Formula: C7H3FN2O3
SMILES: O=C=Nc1ccc(F)c([N+](=O)[O-])c1
Mol. weight [g/mol]:   182.11
CAS: 65303-82-4

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: 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=C65303824&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