2-Nitrophenyl isothiocyanate

Inchi: InChI=1S/C7H4N2O2S/c10-9(11)7-4-2-1-3-6(7)8-5-12/h1-4H
InchiKey: CBWJHIXSVFDERH-UHFFFAOYSA-N
Formula: C7H4N2O2S
SMILES: O=[N+]([O-])c1ccccc1N=C=S
Mol. weight [g/mol]: 180.18
CAS: 2719-30-4

Physical Properties

Property code	Value	Unit	Source
hf	310.56	kJ/mol	Joback Method
hvap	61.15	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.329		Crippen Method
mcvol	120.880	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
tb	689.01	K	Joback Method
tc	980.14	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=C2719304&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