(E)-1-(3-Nitrophenyl)ethanone oxime

Other names: 1-(3-Nitrophenyl)-1-ethanone oxime
Inchi: InChI=1S/C8H8N2O3/c1-6(9-11)7-3-2-4-8(5-7)10(12)13/h2-5,11H,1H3
InchiKey: PDRKZXUNOXCETR-UHFFFAOYSA-N
Formula: C8H8N2O3
SMILES: CC(=NO)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 180.16
CAS: 7471-32-1

Physical Properties

Property code	Value	Unit	Source
hf	-73.95	kJ/mol	Joback Method
hvap	73.00	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.793		Crippen Method
mcvol	128.790	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
rinpol	1807.00		NIST Webbook
tb	734.68	K	Joback Method
tc	975.28	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7471321&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature