(Z)-1-(3-Nitrophenyl)ethanone methoxime

Inchi: InChI=1S/C9H10N2O3/c1-7(10-14-2)8-4-3-5-9(6-8)11(12)13/h3-6H,1-2H3
InchiKey: POQRLGFLWILFNI-UHFFFAOYSA-N
Formula: C9H10N2O3
SMILES: CON=C(C)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 194.19

Physical Properties

Property code	Value	Unit	Source
hf	-74.58	kJ/mol	Joback Method
hvap	60.96	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	1.965		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
rinpol	1579.00		NIST Webbook
rinpol	1579.00		NIST Webbook
tb	687.80	K	Joback Method
tc	942.63	K	Joback Method

Sources

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=U373227&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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