(Z)-1-(4-Methoxy-3-nitro-phenyl)ethanone methoxime

Other names: (Z)-1-(4-Methoxy-3-nitrophenyl)-N-methoxy-ethanimine
Inchi: InChI=1S/C10H12N2O4/c1-7(11-16-3)8-4-5-10(15-2)9(6-8)12(13)14/h4-6H,1-3H3
InchiKey: KDBIODILSHUMOL-UHFFFAOYSA-N
Formula: C10H12N2O4
SMILES: CON=C(C)c1ccc(OC)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 224.21

Physical Properties

Property code	Value	Unit	Source
hf	-238.91	kJ/mol	Joback Method
hvap	66.26	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	1.974		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
rinpol	1806.00		NIST Webbook
rinpol	1806.00		NIST Webbook
tb	738.08	K	Joback Method
tc	983.92	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=U373324&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