(E)-1-(4-Methoxy-3-nitrophenyl)ethanone oxime

Inchi: InChI=1S/C9H10N2O4/c1-6(10-12)7-3-4-9(15-2)8(5-7)11(13)14/h3-5,12H,1-2H3
InchiKey: MKNWFYYUMNOMMS-UHFFFAOYSA-N
Formula: C9H10N2O4
SMILES: COc1ccc(C(C)=NO)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 210.19
CAS: 149773-91-1

Physical Properties

Property code	Value	Unit	Source
hf	-238.28	kJ/mol	Joback Method
hvap	78.30	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.802		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook
tb	784.96	K	Joback Method
tc	1018.66	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C149773911&Units=SI

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