

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

Other names:	E-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	1878.00		NIST Webbook
rinpol	1878.00		NIST Webbook
tb	738.08	K	Joback Method
tc	983.92	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U373328&Units=SI

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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