

Acetophenone, 4-hydroxy-3-methoxy, O-methyloxime

Inchi:	InChI=1S/C10H13NO3/c1-7(11-14-3)8-4-5-9(12)10(6-8)13-2/h4-6,12H,1-3H3/b11-7-
InchiKey:	RDXVUAUDVFNMGC-XFFZJAGNSA-N
Formula:	C10H13NO3
SMILES:	CON=C(C)c1ccc(O)c(OC)c1
Mol. weight [g/mol]:	195.22

Physical Properties

Property code	Value	Unit	Source
hf	-393.99	kJ/mol	Joback Method
hvap	62.02	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.771		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	2931.34	kPa	Joback Method
rinpol	1703.00		NIST Webbook
tb	661.88	K	Joback Method
tc	894.94	K	Joback Method

Sources

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=R99923&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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