

Acetophenone, 4'-methoxy-, oxime

Other names:	Ethanone, 1-(4-methoxyphenyl)-, oxime 1-(4-Methoxyphenyl)ethanone oxime
Inchi:	InChI=1S/C9H11NO2/c1-7(10-11)8-3-5-9(12-2)6-4-8/h3-6,11H,1-2H3
InchiKey:	XXOHMWCSTKXDLH-UHFFFAOYSA-N
Formula:	C9H11NO2
SMILES:	COc1ccc(C(C)=NO)cc1
Mol. weight [g/mol]:	165.19
CAS:	2475-92-5

Physical Properties

Property code	Value	Unit	Source
hf	-216.05	kJ/mol	Joback Method
hvap	61.05	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.893		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
rinpol	1625.00		NIST Webbook
tb	628.14	K	Joback Method
tc	841.24	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=C2475925&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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