

Ethanone, 1-phenyl-, oxime

Other names:	Acetophenone, oxime
Inchi:	InChI=1S/C8H9NO/c1-7(9-10)8-5-3-2-4-6-8/h2-6,10H,1H3
InchiKey:	JHNRZXQVBKRYKN-UHFFFAOYSA-N
Formula:	C8H9NO
SMILES:	CC(=NO)c1ccccc1
Mol. weight [g/mol]:	135.16
CAS:	613-91-2

Physical Properties

Property code	Value	Unit	Source
chs	-4414.00	kJ/mol	NIST Webbook
hf	-51.72	kJ/mol	Joback Method
hfs	-41.00	kJ/mol	NIST Webbook
hvap	55.75	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.885		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1310.00		NIST Webbook
tb	577.86	K	Joback Method
tc	796.25	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C613912&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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