

2-Pentanone, O-methyloxime

Inchi:	InChI=1S/C6H13NO/c1-4-5-6(2)7-8-3/h4-5H2,1-3H3
InchiKey:	CMUPRWBXGFPVTG-UHFFFAOYSA-N
Formula:	C6H13NO
SMILES:	CCCC(C)=NOC
Mol. weight [g/mol]:	115.17
CAS:	31377-00-1

Physical Properties

Property code	Value	Unit	Source
hf	-226.96	kJ/mol	Joback Method
hvap	34.75	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.809		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	781.00		NIST Webbook
tb	435.66	K	Joback Method
tc	626.47	K	Joback Method

Sources

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=C31377001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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