

2-Butanone, 3-methyl-, oxime

Inchi: InChI=1S/C5H11NO/c1-4(2)5(3)6-7/h4,7H,1-3H3
InchiKey: HZCRFUPEBRNAAI-UHFFFAOYSA-N
Formula: C5H11NO
SMILES: CC(=NO)C(C)C
Mol. weight [g/mol]: 101.15
CAS: 600-20-4

Physical Properties

Property code	Value	Unit	Source
hf	-231.61	kJ/mol	Joback Method
hvap	46.41	kJ/mol	Joback Method
log10ws	-0.49		Crippen Method
logp	1.492		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	848.00		NIST Webbook
rinpol	848.00		NIST Webbook
tb	482.10	K	Joback Method
tc	670.37	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C600204&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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