

2-Butanone, 3,3-dimethyl-, oxime

Inchi: InChI=1S/C6H13NO/c1-5(7-8)6(2,3)4/h8H,1-4H3
InchiKey: UNSDDJQNHCSVSW-UHFFFAOYSA-N
Formula: C6H13NO
SMILES: CC(=NO)C(C)(C)C
Mol. weight [g/mol]: 115.17
CAS: 2475-93-6

Physical Properties

Property code	Value	Unit	Source
hf	-255.72	kJ/mol	Joback Method
hvap	47.73	kJ/mol	Joback Method
log10ws	-0.91		Crippen Method
logp	1.883		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
rinpol	938.00		NIST Webbook
rinpol	938.00		NIST Webbook
tb	502.19	K	Joback Method
tc	695.67	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=C2475936&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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
ri_{npol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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