

Butanal, 3-methyl-, oxime

Other names:	3-Methylbutanal oxime 3-methylbutyraldehyde oxime 3)Methyl-butyl-aldoxime
Inchi:	InChI=1S/C5H11NO/c1-5(2)3-4-6-7/h4-5,7H,3H2,1-2H3
InchiKey:	JAUPRNSQRRCCRR-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CC(C)CC=NO
Mol. weight [g/mol]:	101.15
CAS:	626-90-4

Physical Properties

Property code	Value	Unit	Source
hf	-221.82	kJ/mol	Joback Method
hvap	46.33	kJ/mol	Joback Method
log10ws	-0.49		Crippen Method
logp	1.492		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	858.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	870.00		NIST Webbook
tb	482.22	K	Joback Method
tc	667.10	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C626904&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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