

4-Methyl-3-penten-2-one, O-ethyloxime, anty

Inchi: InChI=1S/C8H15NO/c1-5-10-9-8(4)6-7(2)3/h6H,5H2,1-4H3/b9-8+
InchiKey: LKCIEPVYJASXJH-CMDGGGOBGSA-N
Formula: C8H15NO
SMILES: CCON=C(C)C=C(C)C
Mol. weight [g/mol]: 141.21

Physical Properties

Property code	Value	Unit	Source
hf	-160.81	kJ/mol	Joback Method
hvap	39.24	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.365		Crippen Method
mcvol	130.830	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpola	972.00		NIST Webbook
rinpola	972.00		NIST Webbook
tb	485.46	K	Joback Method
tc	684.88	K	Joback Method

Sources

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=R315774&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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