

3-Pentanone oxime

Inchi:	InChI=1S/C5H11NO/c1-3-5(4-2)6-7/h7H,3-4H2,1-2H3
InchiKey:	NAQQTJZRCYNBRX-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CCC(CC)=NO
Mol. weight [g/mol]:	101.15
CAS:	1188-11-0

Physical Properties

Property code	Value	Unit	Source
hf	-226.33	kJ/mol	Joback Method
hvap	46.80	kJ/mol	Joback Method
log10ws	-0.73		Crippen Method
logp	1.637		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
tb	482.54	K	Joback Method
tc	666.81	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	55.80	kJ/mol	371.50	NIST Webbook

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=C1188110&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
h_{vapt}:	Enthalpy of vaporization at a given temperature
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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