

3-Hepten-2-one, 3-methyl-

Other names:	n-C ₃ H ₇ CH=C(CH ₃)C(=O)CH ₃
Inchi:	InChI=1S/C ₈ H ₁₄ O/c1-4-5-6-7(2)8(3)9/h6H,4-5H ₂ ,1-3H ₃ /b7-6+
InchiKey:	IZBMUZVSTLWUTH-VOTSOKGWSA-N
Formula:	C ₈ H ₁₄ O
SMILES:	CCCC=C(C)C(C)=O
Mol. weight [g/mol]:	126.20
CAS:	39899-08-6

Physical Properties

Property code	Value	Unit	Source
gf	-40.77	kJ/mol	Joback Method
hf	-213.60	kJ/mol	Joback Method
hfus	16.97	kJ/mol	Joback Method
hvap	40.19	kJ/mol	Joback Method
ie	9.22	eV	NIST Webbook
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
tb	440.35	K	Joback Method
tc	627.87	K	Joback Method
tf	210.81	K	Joback Method
vc	0.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.66	J/mol×K	440.35	Joback Method
cpg	252.05	J/mol×K	471.60	Joback Method
cpg	263.86	J/mol×K	502.86	Joback Method
cpg	275.09	J/mol×K	534.11	Joback Method
cpg	285.78	J/mol×K	565.36	Joback Method
cpg	295.94	J/mol×K	596.61	Joback Method
cpg	305.60	J/mol×K	627.87	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=C39899086&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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