

1-Hepten-6-one, 2-methyl-

Other names:	6-Methyl-6-hepten-2-one 6-Methylhept-6-en-2-one 6-Hepten-2-one, 6-methyl-
Inchi:	InChI=1S/C8H14O/c1-7(2)5-4-6-8(3)9/h1,4-6H2,2-3H3
InchiKey:	FMCHGBFGIKQNCT-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	C=C(C)CCCC(C)=O
Mol. weight [g/mol]:	126.20
CAS:	10408-15-8

Physical Properties

Property code	Value	Unit	Source
gf	-33.15	kJ/mol	Joback Method
hf	-205.39	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	39.56	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	966.00		NIST Webbook
rinpol	1013.00		NIST Webbook
ripol	1300.00		NIST Webbook
tb	432.87	K	Joback Method
tc	615.30	K	Joback Method
tf	214.13	K	Joback Method
vc	0.471	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.45	J/mol×K	432.87	Joback Method
cpg	251.55	J/mol×K	463.28	Joback Method
cpg	263.12	J/mol×K	493.68	Joback Method

cpg	274.17	J/mol×K	524.09	Joback Method
cpg	284.73	J/mol×K	554.49	Joback Method
cpg	294.80	J/mol×K	584.90	Joback Method
cpg	304.41	J/mol×K	615.30	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=C10408158&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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