

3-Hepten-2-one, 5-methyl-

Other names:	5-Methyl-3-hepten-2-one
Inchi:	InChI=1S/C8H14O/c1-4-7(2)5-6-8(3)9/h5-7H,4H2,1-3H3/b6-5+
InchiKey:	QDUQNQQMHZNNTG-AATRIKPKSA-N
Formula:	C8H14O
SMILES:	CCC(C)C=CC(C)=O
Mol. weight [g/mol]:	126.20
CAS:	5090-16-4

Physical Properties

Property code	Value	Unit	Source
gf	-34.66	kJ/mol	Joback Method
hf	-209.09	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	39.72	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.178		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
tb	440.03	K	Joback Method
tc	628.20	K	Joback Method
tf	209.77	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.81	J/mol×K	440.03	Joback Method
cpg	252.37	J/mol×K	471.39	Joback Method
cpg	264.33	J/mol×K	502.75	Joback Method
cpg	275.70	J/mol×K	534.12	Joback Method
cpg	286.51	J/mol×K	565.48	Joback Method
cpg	296.79	J/mol×K	596.84	Joback Method
cpg	306.55	J/mol×K	628.20	Joback Method
dvisc	0.0063735	Pa×s	209.77	Joback Method

dvisc	0.0024014	Pa×s	248.15	Joback Method
dvisc	0.0011752	Pa×s	286.52	Joback Method
dvisc	0.0006809	Pa×s	324.90	Joback Method
dvisc	0.0004427	Pa×s	363.28	Joback Method
dvisc	0.0003125	Pa×s	401.65	Joback Method
dvisc	0.0002344	Pa×s	440.03	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=C5090164&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mccvol:	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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