

5-Hexen-2-one, 5-methyl-3-ethenyl

Inchi:	InChI=1S/C8H12O/c1-4-6-8(5-2)7(3)9/h4-5,8H,1-2,6H2,3H3
InchiKey:	OOVROPCQEWXDEX-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	C=CCC(C=C)C(C)=O
Mol. weight [g/mol]:	124.18

Physical Properties

Property code	Value	Unit	Source
gf	60.80	kJ/mol	Joback Method
hf	-75.45	kJ/mol	Joback Method
hfus	11.99	kJ/mol	Joback Method
hvap	38.42	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.954		Crippen Method
mcvol	116.550	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	874.00		NIST Webbook
tb	429.23	K	Joback Method
tc	616.17	K	Joback Method
tf	211.33	K	Joback Method
vc	0.446	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.77	J/mol×K	429.23	Joback Method
cpg	276.54	J/mol×K	585.02	Joback Method
cpg	267.03	J/mol×K	553.86	Joback Method
cpg	257.02	J/mol×K	522.70	Joback Method
cpg	246.49	J/mol×K	491.54	Joback Method
cpg	235.41	J/mol×K	460.39	Joback Method
cpg	285.55	J/mol×K	616.17	Joback Method
dvisc	0.0002783	Paxs	429.23	Joback Method
dvisc	0.0003617	Paxs	392.91	Joback Method

dvisc	0.0004958	Paxs	356.60	Joback Method
dvisc	0.0007302	Paxs	320.28	Joback Method
dvisc	0.0011873	Paxs	283.96	Joback Method
dvisc	0.0022265	Paxs	247.65	Joback Method
dvisc	0.0051821	Paxs	211.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R72468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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