1-Hexen-3-one

Other names:	Propyl vinyl ketone
	Vinyl propyl ketone
	hex-1-en-3-one
Inchi:	InChI=1S/C6H10O/c1-3-5-6(7)4-2/h4H,2-3,5H2,1H3
InchiKey:	JTHNLKXLWOXOQK-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	C=CC(=O)CCC
Mol. weight [g/mol]:	98.14
CAS:	1629-60-3

Physical Properties

Property code	Value	Unit	Source
gf	-41.44	kJ/mol	Joback Method
hf	-154.32	kJ/mol	Joback Method
hfus	11.62	kJ/mol	Joback Method
hvap	35.03	kJ/mol	Joback Method
log10ws	-0.83		Aqueous Solubility Prediction Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	747.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	784.00		NIST Webbook

rinpol	777.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	775.00		NIST Webbook
ripol	1087.00		NIST Webbook
ripol	1120.00		NIST Webbook
ripol	1103.00		NIST Webbook
ripol	1096.00		NIST Webbook
ripol	1092.00		NIST Webbook
ripol	1101.00		NIST Webbook
ripol	1101.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1086.00		NIST Webbook
ripol	1106.00		NIST Webbook
ripol	1096.00		NIST Webbook
ripol	1081.00		NIST Webbook
ripol	1081.00		NIST Webbook
ripol	1095.00		NIST Webbook
ripol	1096.00		NIST Webbook
ripol	1096.00		NIST Webbook
ripol	1091.00		NIST Webbook
ripol	1093.00		NIST Webbook
ripol	1099.00		NIST Webbook
ripol	1100.00		NIST Webbook
ripol	1087.00		NIST Webbook
ripol	1086.00		NIST Webbook
tb	387.23	K	Joback Method
tc	568.55	K	Joback Method
tf	205.55	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.39	J/mol×K	387.23	Joback Method

cpg	172.83	J/mol×K	417.45	Joback Method
cpg	181.86	J/mol×K	447.67	Joback Method
cpg	190.50	J/mol×K	477.89	Joback Method
cpg	198.76	J/mol×K	508.11	Joback Method
cpg	206.65	J/mol×K	538.33	Joback Method
cpg	214.18	J/mol×K	568.55	Joback Method
dvisc	0.0032665	Pa×s	205.55	Joback Method
dvisc	0.0016885	Pa×s	235.83	Joback Method
dvisc	0.0010142	Pa×s	266.11	Joback Method
dvisc	0.0006761	Pa×s	296.39	Joback Method
dvisc	0.0004858	Pa×s	326.67	Joback Method
dvisc	0.0003693	Pa×s	356.95	Joback Method
dvisc	0.0002930	Pa×s	387.23	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1629603&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
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