3-Hexen-2-one

Other names: 1-Butenyl methyl ketone
Hex-3-en-2-one
Methyl 1-butenyl ketone
Inchi: InChI=1S/C6H10O/c1-3-4-5-6(2)7/h4-5H,3H2,1-2H3
InchiKey: LPCWMYHBLXLJJQ-UHFFFAOYSA-N
Formula: C6H10O
SMILES: CCC=CC(C)=O
Mol. weight [g/mol]: 98.14
CAS: 763-93-9

Physical Properties

Property code	Value	Unit	Source
gf	-49.06	kJ/mol	Joback Method
hf	-162.53	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	35.65	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	819.00		NIST Webbook
rinpol	813.00		NIST Webbook
rinpol	834.00		NIST Webbook
rinpol	845.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	834.00		NIST Webbook
ripol	1211.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1218.00		NIST Webbook
ripol	1209.00		NIST Webbook
ripol	1218.00		NIST Webbook
tb	394.71	K	Joback Method
tc	581.55	K	Joback Method
tf	202.23	K	Joback Method

vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.73	J/mol×K	394.71	Joback Method
cpg	172.50	J/mol×K	425.85	Joback Method
cpg	181.81	J/mol×K	456.99	Joback Method
cpg	190.67	J/mol×K	488.13	Joback Method
cpg	199.09	J/mol×K	519.27	Joback Method
cpg	207.09	J/mol×K	550.41	Joback Method
cpg	214.70	J/mol×K	581.55	Joback Method
dvisc	0.0034897	Pa×s	202.23	Joback Method
dvisc	0.0016596	Pa×s	234.31	Joback Method
dvisc	0.0009440	Pa×s	266.39	Joback Method
dvisc	0.0006062	Pa×s	298.47	Joback Method
dvisc	0.0004242	Pa×s	330.55	Joback Method
dvisc	0.0003162	Pa×s	362.63	Joback Method
dvisc	0.0002472	Pa×s	394.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47830e+01
Coeff. B	-3.61681e+03
Coeff. C	-5.60060e+01
Temperature range (K), min.	305.52
Temperature range (K), max.	437.87

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C763939&Units=SI

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
pvap:	Vapor 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