5-Hexen-2-one

Other names:	1-Hexen-5-one
	5-Hexene-2-one
	Allylacetone
	hex-5-en-2-one
Inchi:	InChI=1S/C6H10O/c1-3-4-5-6(2)7/h3H,1,4-5H2,2H3
InchiKey:	RNDVGJZUHCKENF-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	C=CCCC(C)=O
Mol. weight [g/mol]:	98.14
CAS:	109-49-9

Physical Properties

Property code	Value	Unit	Source
chl	-3766.00	kJ/mol	NIST Webbook
chl	-3589.00	kJ/mol	NIST Webbook
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
ie	9.50	eV	NIST Webbook
log10ws	-1.47		Crippen 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	737.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	745.00		NIST Webbook
rinpol	744.00		NIST Webbook
ripol	1138.00		NIST Webbook
ripol	1135.00		NIST Webbook
ripol	1135.00		NIST Webbook
tb	402.70	K	NIST Webbook
tb	401.00	K	NIST Webbook
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	181.86	J/mol×K	447.67	Joback Method
cpg	214.18	J/mol×K	568.55	Joback Method
cpg	206.65	J/mol×K	538.33	Joback Method
cpg	198.76	J/mol×K	508.11	Joback Method
cpg	190.50	J/mol×K	477.89	Joback Method
cpg	163.39	J/mol×K	387.23	Joback Method
cpg	172.83	J/mol×K	417.45	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	0.0032665	Pa×s	205.55	Joback Method
dvisc	0.0002930	Pa×s	387.23	Joback Method
hvapt	34.60	kJ/mol	505.00	NIST Webbook
hvapt	33.50 ± 0.60	kJ/mol	378.50	NIST Webbook
hvapt	36.60 ± 0.30	kJ/mol	378.50	NIST Webbook
hvapt	39.40 ± 0.20	kJ/mol	378.50	NIST Webbook
hvapt	42.10 ± 0.10	kJ/mol	378.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	342.20	K	13.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47920e+01

Coeff. B	-3.53956e+03
Coeff. C	-5.30870e+01
Temperature range (K), min.	297.12
Temperature range (K), max.	426.44

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109499&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume