

4-Hexen-2-one

Other names:	2-Hexen-5-one Acetone, methylallyl Methylallyl acetone
Inchi:	InChI=1S/C6H10O/c1-3-4-5-6(2)7/h3-4H,5H2,1-2H3/b4-3+
InchiKey:	YRXUQYBLFBZHNE-ONEGZZNKSA-N
Formula:	C6H10O
SMILES:	CC=CCC(C)=O
Mol. weight [g/mol]:	98.14
CAS:	25659-22-7

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
tb	409.20	K	NIST Webbook
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/molxK	394.71	Joback Method
cpg	172.50	J/molxK	425.85	Joback Method
cpg	181.81	J/molxK	456.99	Joback Method
cpg	190.67	J/molxK	488.13	Joback Method
cpg	199.09	J/molxK	519.27	Joback Method
cpg	207.09	J/molxK	550.41	Joback Method

cpg	214.70	J/mol×K	581.55	Joback Method
dvisc	0.0034897	Paxs	202.23	Joback Method
dvisc	0.0016596	Paxs	234.31	Joback Method
dvisc	0.0009440	Paxs	266.39	Joback Method
dvisc	0.0006062	Paxs	298.47	Joback Method
dvisc	0.0004242	Paxs	330.55	Joback Method
dvisc	0.0003162	Paxs	362.63	Joback Method
dvisc	0.0002472	Paxs	394.71	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38329e+01
Coeff. B	-3.28781e+03
Coeff. C	-5.23920e+01
Temperature range (K), min.	295.12
Temperature range (K), max.	438.22

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25659227&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/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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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