

5-Hexen-3-one

Inchi:	InChI=1S/C6H10O/c1-3-5-6(7)4-2/h3H,1,4-5H2,2H3
InchiKey:	RUJLJMUWUVTHEU-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	C=CCC(=O)CC
Mol. weight [g/mol]:	98.14
CAS:	24253-30-3

Physical Properties

Property code	Value	Unit	Source
chl	-3591.00	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
log10ws	-1.47		Crippen Method
logp	1.542		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	387.23	K	Joback Method
tc	568.55	K	Joback Method
tf	205.55	K	Joback Method
vc	0.358	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.39	J/molxK	387.23	Joback Method
cpg	172.83	J/molxK	417.45	Joback Method
cpg	181.86	J/molxK	447.67	Joback Method
cpg	190.50	J/molxK	477.89	Joback Method
cpg	198.76	J/molxK	508.11	Joback Method
cpg	206.65	J/molxK	538.33	Joback Method
cpg	214.18	J/molxK	568.55	Joback Method
dvisc	0.0032665	Paxs	205.55	Joback Method

dvisc	0.0016885	Paxs	235.83	Joback Method
dvisc	0.0010142	Paxs	266.11	Joback Method
dvisc	0.0006761	Paxs	296.39	Joback Method
dvisc	0.0004858	Paxs	326.67	Joback Method
dvisc	0.0003693	Paxs	356.95	Joback Method
dvisc	0.0002930	Paxs	387.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24253303&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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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