

3-hydroxy-1-hexen-4-one

Inchi:	InChI=1S/C6H10O2/c1-3-5(7)6(8)4-2/h3,5,7H,1,4H2,2H3
InchiKey:	BFAZWULGRMBHPB-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	C=CC(O)C(=O)CC
Mol. weight [g/mol]:	114.14

Physical Properties

Property code	Value	Unit	Source
gf	-180.70	kJ/mol	Joback Method
hf	-311.83	kJ/mol	Joback Method
hfus	12.18	kJ/mol	Joback Method
hvap	51.32	kJ/mol	Joback Method
log10ws	-0.84		Crippen Method
logp	0.512		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
ripol	1453.00		NIST Webbook
ripol	1453.00		NIST Webbook
tb	478.97	K	Joback Method
tc	657.28	K	Joback Method
tf	251.37	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.84	J/molxK	478.97	Joback Method
cpg	215.35	J/molxK	508.69	Joback Method
cpg	223.47	J/molxK	538.41	Joback Method
cpg	231.22	J/molxK	568.12	Joback Method
cpg	238.60	J/molxK	597.84	Joback Method
cpg	245.62	J/molxK	627.56	Joback Method
cpg	252.30	J/molxK	657.28	Joback Method
dvisc	0.0411915	Paxs	251.37	Joback Method

dvisc	0.0094923	Paxs	289.30	Joback Method
dvisc	0.0030741	Paxs	327.24	Joback Method
dvisc	0.0012583	Paxs	365.17	Joback Method
dvisc	0.0006094	Paxs	403.10	Joback Method
dvisc	0.0003343	Paxs	441.04	Joback Method
dvisc	0.0002017	Paxs	478.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R241084&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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