4-hydroxy-1-hexen-3-one

Inchi: InChI=1S/C6H10O2/c1-3-5(7)6(8)4-2/h3,6,8H,1,4H2,2H3
InchiKey: ZWFSKVZACXTELI-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	1430.00		NIST Webbook
ripol	1430.00		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/mol×K	478.97	Joback Method
cpg	245.62	J/mol×K	627.56	Joback Method
cpg	238.60	J/mol×K	597.84	Joback Method
cpg	231.22	J/mol×K	568.12	Joback Method
cpg	223.47	J/mol×K	538.41	Joback Method
cpg	215.35	J/mol×K	508.69	Joback Method
cpg	252.30	J/mol×K	657.28	Joback Method
dvisc	0.0002017	Pa×s	478.97	Joback Method

dvisc	0.0003343	Pa×s	441.04	Joback Method
dvisc	0.0006094	Pa×s	403.10	Joback Method
dvisc	0.0012583	Pa×s	365.17	Joback Method
dvisc	0.0030741	Pa×s	327.24	Joback Method
dvisc	0.0094923	Pa×s	289.30	Joback Method
dvisc	0.0411915	Pa×s	251.37	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=R241202&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