3-hydroxy-(E)-4-hexen-2-one

Inchi: InChI=1S/C6H10O2/c1-3-4-6(8)5(2)7/h3-4,6,8H,1-2H3/b4-3+
InchiKey: SNHRCGORDKLMQV-ONEGZZNKSA-N
Formula: C6H10O2
SMILES: CC=CC(O)C(C)=O
Mol. weight [g/mol]: 114.14

Physical Properties

Property code	Value	Unit	Source
gf	-188.32	kJ/mol	Joback Method
hf	-320.04	kJ/mol	Joback Method
hfus	13.66	kJ/mol	Joback Method
hvap	51.94	kJ/mol	Joback Method
log10ws	-0.84		Crippen Method
logp	0.512		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
ripol	1481.00		NIST Webbook
tb	486.45	K	Joback Method
tc	669.30	K	Joback Method
tf	248.05	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.34	J/mol×K	486.45	Joback Method
cpg	215.01	J/mol×K	516.92	Joback Method
cpg	223.25	J/mol×K	547.40	Joback Method
cpg	231.07	J/mol×K	577.87	Joback Method
cpg	238.49	J/mol×K	608.35	Joback Method
cpg	245.53	J/mol×K	638.82	Joback Method
cpg	252.21	J/mol×K	669.30	Joback Method
dvisc	0.0452390	Pa×s	248.05	Joback Method
dvisc	0.0092323	Pa×s	287.78	Joback Method

dvisc	0.0027706	Pa×s	327.52	Joback Method
dvisc	0.0010788	Pa×s	367.25	Joback Method
dvisc	0.0005050	Pa×s	406.98	Joback Method
dvisc	0.0002706	Pa×s	446.72	Joback Method
dvisc	0.0001605	Pa×s	486.45	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R241113&Units=SI

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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