

3-Hydroxy-4-hexenoic acid, ethyl ester

Inchi:	InChI=1S/C8H14O3/c1-3-5-7(9)6-8(10)11-4-2/h3,5,7,9H,4,6H2,1-2H3/b5-3+
InchiKey:	PCOMBRWRJCHFEGG-HWKANZROSA-N
Formula:	C8H14O3
SMILES:	CC=CC(O)CC(=O)OCC
Mol. weight [g/mol]:	158.19
CAS:	20316-32-9

Physical Properties

Property code	Value	Unit	Source
gf	-276.48	kJ/mol	Joback Method
hf	-493.54	kJ/mol	Joback Method
hfus	20.03	kJ/mol	Joback Method
hvap	58.81	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	0.877		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	554.63	K	Joback Method
tc	733.07	K	Joback Method
tf	292.82	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.53	J/mol×K	554.63	Joback Method
cpg	362.44	J/mol×K	703.33	Joback Method
cpg	353.74	J/mol×K	673.59	Joback Method
cpg	344.62	J/mol×K	643.85	Joback Method
cpg	335.05	J/mol×K	614.11	Joback Method
cpg	325.03	J/mol×K	584.37	Joback Method
cpg	370.71	J/mol×K	733.07	Joback Method
dvisc	0.0000864	Pa×s	554.63	Joback Method
dvisc	0.0001407	Pa×s	511.00	Joback Method

dvisc	0.0002508	Pa×s	467.36	Joback Method
dvisc	0.0005039	Pa×s	423.73	Joback Method
dvisc	0.0011880	Pa×s	380.09	Joback Method
dvisc	0.0034988	Pa×s	336.46	Joback Method
dvisc	0.0142179	Pa×s	292.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20316329&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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