

Hexanoic acid, 3-hydroxy-, ethyl ester

Other names:	Ethyl hydroxy-3-hexanoate ethyl 3-hydroxyhexanoate
Inchi:	InChI=1S/C8H16O3/c1-3-5-7(9)6-8(10)11-4-2/h7,9H,3-6H2,1-2H3
InchiKey:	LYRIITRHDCNUHV-UHFFFAOYSA-N
Formula:	C8H16O3
SMILES:	CCCC(O)CC(=O)OCC
Mol. weight [g/mol]:	160.21
CAS:	2305-25-1

Physical Properties

Property code	Value	Unit	Source
gf	-356.70	kJ/mol	Joback Method
hf	-610.76	kJ/mol	Joback Method
hfus	19.83	kJ/mol	Joback Method
hvap	61.90 ± 0.60	kJ/mol	NIST Webbook
log10ws	-1.41		Crippen Method
logp	1.101		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1129.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1133.00		NIST Webbook

rinpol	1134.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1126.00	NIST Webbook
rinpol	1121.00	NIST Webbook
rinpol	1133.00	NIST Webbook
rinpol	1125.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1122.00	NIST Webbook
rinpol	1124.00	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1157.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1126.00	NIST Webbook
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rinpol	1133.00	NIST Webbook
rinpol	1133.00	NIST Webbook
ripol	1690.00	NIST Webbook
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ripol	1652.00	NIST Webbook
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ripol	1675.00	NIST Webbook
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ripol	1675.00	NIST Webbook
ripol	1674.00	NIST Webbook
ripol	1650.00	NIST Webbook
ripol	1663.00	NIST Webbook
ripol	1675.00	NIST Webbook
ripol	1666.00	NIST Webbook
ripol	1675.00	NIST Webbook
ripol	1671.00	NIST Webbook
ripol	1677.00	NIST Webbook
ripol	1674.00	NIST Webbook
ripol	1664.00	NIST Webbook
ripol	1663.00	NIST Webbook

ripol	1664.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1661.00		NIST Webbook
tb	550.47	K	Joback Method
tc	722.09	K	Joback Method
tf	297.90	K	Joback Method
vc	0.520	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.29	J/molxK	722.09	Joback Method
cpg	333.69	J/molxK	550.47	Joback Method
cpg	344.69	J/molxK	579.07	Joback Method
cpg	355.26	J/molxK	607.68	Joback Method
cpg	365.40	J/molxK	636.28	Joback Method
cpg	375.11	J/molxK	664.88	Joback Method
cpg	384.41	J/molxK	693.49	Joback Method
dvisc	0.0001040	Paxs	550.47	Joback Method
dvisc	0.0141338	Paxs	297.90	Joback Method
dvisc	0.0037547	Paxs	340.00	Joback Method
dvisc	0.0013358	Paxs	382.09	Joback Method
dvisc	0.0005834	Paxs	424.19	Joback Method
dvisc	0.0002959	Paxs	466.28	Joback Method
dvisc	0.0001680	Paxs	508.38	Joback Method
hvapt	61.80	kJ/mol	298.15	Application of correlation-gas chromatography to evaluate the vaporization enthalpy of a component in an equilibrium mixture

Sources

Application of correlation-gas chromatography to evaluate the vaporization enthalpy of a component in an equilibrium mixture: McGowan Method:

<https://www.doi.org/10.1016/j.tca.2005.03.021>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2305251&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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