ethyl 5-hydroxyhexanoate

Other names: Hexanoic acid, 5-hydroxy, ethyl ester
Inchi: InChI=1S/C8H16O3/c1-3-11-8(10)6-4-5-7(2)9/h7,9H,3-6H2,1-2H3
InchiKey: YUQVKXFPYUHIIF-UHFFFAOYSA-N
Formula: C8H16O3
SMILES: CCOC(=O)CCCC(C)O
Mol. weight [g/mol]: 160.21

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	58.85	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.101		Crippen Method
mcvol	136.890	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
ripol	1872.00		NIST Webbook
ripol	1865.00		NIST Webbook
ripol	1848.00		NIST Webbook
ripol	1865.00		NIST Webbook
ripol	1848.00		NIST Webbook
tb	550.47	K	Joback Method
tc	722.09	K	Joback Method
tf	297.90	K	Joback Method
vc	0.520	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.69	J/mol×K	550.47	Joback Method
cpg	344.69	J/mol×K	579.07	Joback Method
cpg	355.26	J/mol×K	607.68	Joback Method
cpg	365.40	J/mol×K	636.28	Joback Method

cpg	375.11	J/mol×K	664.88	Joback Method
cpg	384.41	J/mol×K	693.49	Joback Method
cpg	393.29	J/mol×K	722.09	Joback Method
dvisc	0.0141338	Pa×s	297.90	Joback Method
dvisc	0.0037547	Pa×s	340.00	Joback Method
dvisc	0.0013358	Pa×s	382.09	Joback Method
dvisc	0.0005834	Pa×s	424.19	Joback Method
dvisc	0.0002959	Pa×s	466.28	Joback Method
dvisc	0.0001680	Pa×s	508.38	Joback Method
dvisc	0.0001040	Pa×s	550.47	Joback Method

Sources

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=R289195&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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