Propanoic acid, 2-methyl-, 2-ethyl-3-hydroxyhexyl ester

Other names: 2-Ethyl-3-hydroxyhexyl 2-methylpropanoate
Inchi: InChI=1S/C12H24O3/c1-5-7-11(13)10(6-2)8-15-12(14)9(3)4/h9-11,13H,5-8H2,1-4H3
InchiKey: QQRIGCXMIPFTKR-UHFFFAOYSA-N
Formula: C12H24O3
SMILES: CCCC(O)C(CC)COC(=O)C(C)C
Mol. weight [g/mol]: 216.32
CAS: 74367-31-0

Physical Properties

Property code	Value	Unit	Source
gf	-327.90	kJ/mol	Joback Method
hf	-703.88	kJ/mol	Joback Method
hfus	23.14	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.373		Crippen Method
mcvol	193.250	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	1373.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1373.00		NIST Webbook
tb	641.11	K	Joback Method
tc	814.54	K	Joback Method
tf	312.98	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.49	J/mol×K	641.11	Joback Method
cpg	545.81	J/mol×K	670.01	Joback Method

cpg	559.48	J/mol×K	698.92	Joback Method
cpg	572.52	J/mol×K	727.82	Joback Method
cpg	584.94	J/mol×K	756.73	Joback Method
cpg	596.74	J/mol×K	785.63	Joback Method
cpg	607.94	J/mol×K	814.54	Joback Method
dvisc	0.0166774	Pa×s	312.98	Joback Method
dvisc	0.0029545	Pa×s	367.67	Joback Method
dvisc	0.0008194	Pa×s	422.36	Joback Method
dvisc	0.0003049	Pa×s	477.05	Joback Method
dvisc	0.0001391	Pa×s	531.73	Joback Method
dvisc	0.0000734	Pa×s	586.42	Joback Method
dvisc	0.0000432	Pa×s	641.11	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74367310&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

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume