Hexanoic acid, 3,5,5-trimethyl-, 2-ethylhexyl ester

Inchi: InChI=1S/C17H34O2/c1-7-9-10-15(8-2)13-19-16(18)11-14(3)12-17(4,5)6/h14-15H,7-13H

InchiKey: LCVHZNSIAYNAGX-UHFFFAOYSA-N

Formula: C17H34O2

SMILES: CCCCC(CC)COC(=O)CC(C)CC(C)(C)C

Mol. weight [g/mol]: 270.45

Physical Properties

Property code	Value	Unit	Source
gf	-143.70	kJ/mol	Joback Method
hf	-658.32	kJ/mol	Joback Method
hfus	28.11	kJ/mol	Joback Method
hvap	60.52	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	5.208		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	660.54	K	Joback Method
tc	838.82	K	Joback Method
tf	325.93	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.30	J/mol×K	660.54	Joback Method
cpg	823.25	J/mol×K	809.11	Joback Method
cpg	807.44	J/mol×K	779.39	Joback Method
cpg	790.77	J/mol×K	749.68	Joback Method
cpg	773.21	J/mol×K	719.97	Joback Method
cpg	754.73	J/mol×K	690.25	Joback Method
cpg	838.23	J/mol×K	838.82	Joback Method
dvisc	0.0000799	Pa×s	660.54	Joback Method

dvisc	0.0001148	Pa×s	604.77	Joback Method
dvisc	0.0001776	Pa×s	549.00	Joback Method
dvisc	0.0003031	Pa×s	493.23	Joback Method
dvisc	0.0005928	Pa×s	437.47	Joback Method
dvisc	0.0014107	Pa×s	381.70	Joback Method
dvisc	0.0045159	Pa×s	325.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406822&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume