Hexanoic acid, 3,5,5-trimethyl-, octyl ester

Inchi: InChI=1S/C17H34O2/c1-6-7-8-9-10-11-12-19-16(18)13-15(2)14-17(3,4)5/h15H,6-14H2,1
InchiKey: AFKAUGCQTBKHFR-UHFFFAOYSA-N
Formula: C17H34O2
SMILES: CCCCCCCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 270.45

Physical Properties

Property code	Value	Unit	Source
gf	-141.26	kJ/mol	Joback Method
hf	-653.04	kJ/mol	Joback Method
hfus	31.64	kJ/mol	Joback Method
hvap	60.91	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	5.353		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1296.73	kPa	Joback Method
rinpol	1737.00		NIST Webbook
rinpol	1737.00		NIST Webbook
tb	660.98	K	Joback Method
tc	836.78	K	Joback Method
tf	340.93	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.90	J/mol×K	660.98	Joback Method
cpg	754.03	J/mol×K	690.28	Joback Method
cpg	772.24	J/mol×K	719.58	Joback Method
cpg	789.56	J/mol×K	748.88	Joback Method
cpg	806.02	J/mol×K	778.18	Joback Method
cpg	821.65	J/mol×K	807.48	Joback Method
cpg	836.49	J/mol×K	836.78	Joback Method
dvisc	0.0032553	Pa×s	340.93	Joback Method

dvisc	0.0011797	Pa×s	394.27	Joback Method
dvisc	0.0005445	Pa×s	447.61	Joback Method
dvisc	0.0002963	Pa×s	500.95	Joback Method
dvisc	0.0001813	Pa×s	554.30	Joback Method
dvisc	0.0001209	Pa×s	607.64	Joback Method
dvisc	0.0000861	Pa×s	660.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406059&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

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