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

Inchi: InChI=1S/C18H36O2/c1-6-7-8-9-10-11-12-13-20-17(19)14-16(2)15-18(3,4)5/h16H,6-15H
InchiKey: ZZEAXDKLJQQOJD-UHFFFAOYSA-N
Formula: C18H36O2
SMILES: CCCCCCCCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 284.48

Physical Properties

Property code	Value	Unit	Source
gf	-132.84	kJ/mol	Joback Method
hf	-673.68	kJ/mol	Joback Method
hfus	34.23	kJ/mol	Joback Method
hvap	63.13	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.743		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1211.51	kPa	Joback Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
tb	683.86	K	Joback Method
tc	859.39	K	Joback Method
tf	352.20	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.34	J/mol×K	683.86	Joback Method
cpg	811.79	J/mol×K	713.11	Joback Method
cpg	830.29	J/mol×K	742.37	Joback Method
cpg	847.88	J/mol×K	771.62	Joback Method
cpg	864.60	J/mol×K	800.88	Joback Method
cpg	880.47	J/mol×K	830.13	Joback Method
cpg	895.52	J/mol×K	859.39	Joback Method
dvisc	0.0028839	Pa×s	352.20	Joback Method

dvisc	0.0010384	Pa×s	407.48	Joback Method
dvisc	0.0004772	Pa×s	462.75	Joback Method
dvisc	0.0002589	Pa×s	518.03	Joback Method
dvisc	0.0001581	Pa×s	573.31	Joback Method
dvisc	0.0001052	Pa×s	628.58	Joback Method
dvisc	0.0000748	Pa×s	683.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406060&Units=SI

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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