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

Inchi: InChI=1S/C27H54O2/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-29-26(28)23-
InchiKey: IRPUQPOQLCBARJ-UHFFFAOYSA-N
Formula: C27H54O2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 410.72

Physical Properties

Property code	Value	Unit	Source
gf	-57.06	kJ/mol	Joback Method
hf	-859.44	kJ/mol	Joback Method
hfus	57.54	kJ/mol	Joback Method
hvap	83.17	kJ/mol	Joback Method
log10ws	-9.50		Crippen Method
logp	9.253		Crippen Method
mcvol	398.730	ml/mol	McGowan Method
pc	716.07	kPa	Joback Method
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
tb	889.78	K	Joback Method
tc	1090.17	K	Joback Method
tf	453.63	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.73	J/mol×K	889.78	Joback Method
cpg	1373.80	J/mol×K	923.18	Joback Method
cpg	1395.51	J/mol×K	956.58	Joback Method
cpg	1415.92	J/mol×K	989.98	Joback Method
cpg	1435.12	J/mol×K	1023.38	Joback Method
cpg	1453.17	J/mol×K	1056.78	Joback Method
cpg	1470.13	J/mol×K	1090.17	Joback Method
dvisc	0.0008352	Pa×s	453.63	Joback Method

dvisc	0.0002878	Pa×s	526.32	Joback Method
dvisc	0.0001284	Pa×s	599.01	Joback Method
dvisc	0.0000682	Pa×s	671.70	Joback Method
dvisc	0.0000410	Pa×s	744.40	Joback Method
dvisc	0.0000270	Pa×s	817.09	Joback Method
dvisc	0.0000190	Pa×s	889.78	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=U406069&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume