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

Inchi: InChI=1S/C25H50O2/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-27-24(26)21-23(2)22-25(3,4)5

InchiKey: HJQLXIPVQPEJRY-UHFFFAOYSA-N

Formula: C25H50O2

SMILES: CCCCCCCCCCCCCCCCOC(=O)CC(C)CC(C)(C)C

Mol. weight [g/mol]: 382.66

Physical Properties

Property code	Value	Unit	Source
gf	-73.90	kJ/mol	Joback Method
hf	-818.16	kJ/mol	Joback Method
hfus	52.36	kJ/mol	Joback Method
hvap	78.72	kJ/mol	Joback Method
log10ws	-8.67		Crippen Method
logp	8.473		Crippen Method
mcvol	370.550	ml/mol	McGowan Method
pc	795.73	kPa	Joback Method
rinpol	2546.00		NIST Webbook
rinpol	2546.00		NIST Webbook
tb	844.02	K	Joback Method
tc	1033.52	K	Joback Method
tf	431.09	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1221.43	J/mol×K	844.02	Joback Method
cpg	1319.67	J/mol×K	1001.94	Joback Method
cpg	1302.23	J/mol×K	970.36	Joback Method
cpg	1283.75	J/mol×K	938.77	Joback Method
cpg	1264.15	J/mol×K	907.19	Joback Method
cpg	1243.40	J/mol×K	875.60	Joback Method
cpg	1336.11	J/mol×K	1033.52	Joback Method
dvisc	0.0000261	Pa×s	844.02	Joback Method

dvisc	0.0000370	Pa×s	775.20	Joback Method
dvisc	0.0000562	Pa×s	706.38	Joback Method
dvisc	0.0000931	Pa×s	637.56	Joback Method
dvisc	0.0001746	Pa×s	568.73	Joback Method
dvisc	0.0003892	Pa×s	499.91	Joback Method
dvisc	0.0011204	Pa×s	431.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406067&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