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

Inchi: InChI=1S/C26H52O2/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-28-25(27)22-24(

InchiKey: QBUCOQMZPGBRSL-UHFFFAOYSA-N

Formula: C26H52O2

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

Mol. weight [g/mol]: 396.69

Physical Properties

Property code	Value	Unit	Source
gf	-65.48	kJ/mol	Joback Method
hf	-838.80	kJ/mol	Joback Method
hfus	54.95	kJ/mol	Joback Method
hvap	80.94	kJ/mol	Joback Method
log10ws	-9.09		Crippen Method
logp	8.863		Crippen Method
mcvol	384.640	ml/mol	McGowan Method
pc	754.33	kPa	Joback Method
rinpol	2650.00		NIST Webbook
rinpol	2650.00		NIST Webbook
tb	866.90	K	Joback Method
tc	1061.38	K	Joback Method
tf	442.36	K	Joback Method
vc	1.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.79	J/mol×K	866.90	Joback Method
cpg	1308.28	J/mol×K	899.31	Joback Method
cpg	1329.48	J/mol×K	931.73	Joback Method
cpg	1349.46	J/mol×K	964.14	Joback Method
cpg	1368.28	J/mol×K	996.55	Joback Method
cpg	1386.01	J/mol×K	1028.96	Joback Method
cpg	1402.70	J/mol×K	1061.38	Joback Method
dvisc	0.0009683	Pa×s	442.36	Joback Method

dvisc	0.0003350	Pa×s	513.12	Joback Method
dvisc	0.0001499	Pa×s	583.87	Joback Method
dvisc	0.0000798	Pa×s	654.63	Joback Method
dvisc	0.0000480	Pa×s	725.39	Joback Method
dvisc	0.0000317	Pa×s	796.14	Joback Method
dvisc	0.0000223	Pa×s	866.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406068&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