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

Inchi: InChI=1S/C24H48O2/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-26-23(25)20-22(2)21-2

InchiKey: HSYHGXYSZGDNAR-UHFFFAOYSA-N

Formula: C24H48O2

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

Mol. weight [g/mol]: 368.64

Physical Properties

Property code	Value	Unit	Source
gf	-82.32	kJ/mol	Joback Method
hf	-797.52	kJ/mol	Joback Method
hfus	49.77	kJ/mol	Joback Method
hvap	76.49	kJ/mol	Joback Method
log10ws	-8.25		Crippen Method
logp	8.083		Crippen Method
mcvol	356.460	ml/mol	McGowan Method
pc	840.65	kPa	Joback Method
rinpol	2443.00		NIST Webbook
rinpol	2443.00		NIST Webbook
tb	821.14	K	Joback Method
tc	1006.54	K	Joback Method
tf	419.82	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.72	J/mol×K	821.14	Joback Method
cpg	1254.18	J/mol×K	975.64	Joback Method
cpg	1237.00	J/mol×K	944.74	Joback Method
cpg	1218.82	J/mol×K	913.84	Joback Method
cpg	1199.58	J/mol×K	882.94	Joback Method
cpg	1179.23	J/mol×K	852.04	Joback Method
cpg	1270.39	J/mol×K	1006.54	Joback Method
dvisc	0.0000306	Pa×s	821.14	Joback Method

dvisc	0.0000433	Pa×s	754.25	Joback Method
dvisc	0.0000655	Pa×s	687.37	Joback Method
dvisc	0.0001085	Pa×s	620.48	Joback Method
dvisc	0.0002030	Pa×s	553.59	Joback Method
dvisc	0.0004512	Pa×s	486.71	Joback Method
dvisc	0.0012933	Pa×s	419.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406066&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

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