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

Inchi: InChI=1S/C23H46O2/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-25-22(24)19-21(2)20-23(3

InchiKey: KUGGOUVGKCLGGH-UHFFFAOYSA-N

Formula: C23H46O2

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

Mol. weight [g/mol]: 354.61

Physical Properties

Property code	Value	Unit	Source
gf	-90.74	kJ/mol	Joback Method
hf	-776.88	kJ/mol	Joback Method
hfus	47.18	kJ/mol	Joback Method
hvap	74.26	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	7.693		Crippen Method
mcvol	342.370	ml/mol	McGowan Method
pc	889.47	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
tb	798.26	K	Joback Method
tc	980.37	K	Joback Method
tf	408.55	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1094.71	J/mol×K	798.26	Joback Method
cpg	1189.55	J/mol×K	950.02	Joback Method
cpg	1172.62	J/mol×K	919.66	Joback Method
cpg	1154.71	J/mol×K	889.31	Joback Method
cpg	1135.79	J/mol×K	858.96	Joback Method
cpg	1115.80	J/mol×K	828.61	Joback Method
cpg	1205.56	J/mol×K	980.37	Joback Method
dvisc	0.0000357	Pa×s	798.26	Joback Method

dvisc	0.0000505	Pa×s	733.31	Joback Method
dvisc	0.0000763	Pa×s	668.36	Joback Method
dvisc	0.0001262	Pa×s	603.40	Joback Method
dvisc	0.0002356	Pa×s	538.45	Joback Method
dvisc	0.0005220	Pa×s	473.50	Joback Method
dvisc	0.0014893	Pa×s	408.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406065&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