Hexanoic acid, 3,5,5-trimethyl-, tetradec-4-yl ester

Inchi: InChI=1S/C23H46O2/c1-7-9-10-11-12-13-14-15-17-21(16-8-2)25-22(24)18-20(3)19-23(4

InchiKey: PETXYGCYDLYCGT-UHFFFAOYSA-N

Formula: C23H46O2

SMILES: CCCCCCCCCCC(CCC)OC(=O)CC(C)CC(C)(C)C

Mol. weight [g/mol]: 354.61

Physical Properties

Property code	Value	Unit	Source
gf	-93.18	kJ/mol	Joback Method
hf	-782.16	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	73.88	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	7.691		Crippen Method
mcvol	342.370	ml/mol	McGowan Method
pc	893.73	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	797.82	K	Joback Method
tc	980.78	K	Joback Method
tf	393.55	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1095.14	J/mol×K	797.82	Joback Method
cpg	1116.34	J/mol×K	828.31	Joback Method
cpg	1136.41	J/mol×K	858.81	Joback Method
cpg	1155.41	J/mol×K	889.30	Joback Method
cpg	1173.36	J/mol×K	919.79	Joback Method
cpg	1190.33	J/mol×K	950.29	Joback Method
cpg	1206.35	J/mol×K	980.78	Joback Method
dvisc	0.0019189	Pa×s	393.55	Joback Method

dvisc	0.0005932	Pa×s	460.93	Joback Method
dvisc	0.0002474	Pa×s	528.31	Joback Method
dvisc	0.0001258	Pa×s	595.68	Joback Method
dvisc	0.0000733	Pa×s	663.06	Joback Method
dvisc	0.0000473	Pa×s	730.44	Joback Method
dvisc	0.0000328	Pa×s	797.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406268&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