

Hexanoic acid, 3,5,5-trimethyl-, tetradec-7-yl ester

Inchi:	InChI=1S/C23H46O2/c1-7-9-11-13-15-17-21(16-14-12-10-8-2)25-22(24)18-20(3)19-23(4)
InchiKey:	CTNLVQLBSKKQOV-UHFFFAOYSA-N
Formula:	C23H46O2
SMILES:	CCCCCCCC(CCCCC)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
mvol	342.370	ml/mol	McGowan Method
pc	893.73	kPa	Joback Method
rinpol	2148.00		NIST Webbook
rinpol	2148.00		NIST Webbook
tb	797.82	K	Joback Method
tc	980.78	K	Joback Method
tf	393.55	K	Joback Method
vc	1.325	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0005932	Paxs	460.93	Joback Method
dvisc	0.0002474	Paxs	528.31	Joback Method
dvisc	0.0001258	Paxs	595.68	Joback Method
dvisc	0.0000733	Paxs	663.06	Joback Method
dvisc	0.0000473	Paxs	730.44	Joback Method
dvisc	0.0000328	Paxs	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=U406271&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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