

Hexanoic acid, 3,5,5-trimethyl-, pentadec-3-yl ester

Inchi:	InChI=1S/C24H48O2/c1-7-9-10-11-12-13-14-15-16-17-18-22(8-2)26-23(25)19-21(3)20-2
InchiKey:	KTKAZRHNUULYPK-UHFFFAOYSA-N
Formula:	C24H48O2
SMILES:	CCCCCCCCCCCC(CC)OC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]:	368.64

Physical Properties

Property code	Value	Unit	Source
gf	-84.76	kJ/mol	Joback Method
hf	-802.80	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	76.10	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	8.082		Crippen Method
mvol	356.460	ml/mol	McGowan Method
pc	844.56	kPa	Joback Method
rinpol	2307.00		NIST Webbook
rinpol	2307.00		NIST Webbook
tb	820.70	K	Joback Method
tc	1006.64	K	Joback Method
tf	404.82	K	Joback Method
vc	1.381	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.15	J/molxK	820.70	Joback Method
cpg	1254.76	J/molxK	975.65	Joback Method
cpg	1237.59	J/molxK	944.66	Joback Method
cpg	1219.39	J/molxK	913.67	Joback Method
cpg	1200.12	J/molxK	882.68	Joback Method
cpg	1179.72	J/molxK	851.69	Joback Method
cpg	1270.97	J/molxK	1006.64	Joback Method
dvisc	0.0000281	Paxs	820.70	Joback Method

dvisc	0.0000404	Paxs	751.39	Joback Method
dvisc	0.0000628	Paxs	682.07	Joback Method
dvisc	0.0001078	Paxs	612.76	Joback Method
dvisc	0.0002122	Paxs	543.45	Joback Method
dvisc	0.0005093	Paxs	474.13	Joback Method
dvisc	0.0016496	Paxs	404.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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