

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

Inchi:	InChI=1S/C22H44O2/c1-6-7-8-9-10-11-12-13-14-15-16-17-24-21(23)18-20(2)19-22(3,4)5
InchiKey:	NRKCZQACTUADPZ-UHFFFAOYSA-N
Formula:	C22H44O2
SMILES:	CCCCCCCCCCCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]:	340.58

Physical Properties

Property code	Value	Unit	Source
gf	-99.16	kJ/mol	Joback Method
hf	-756.24	kJ/mol	Joback Method
hfus	44.59	kJ/mol	Joback Method
hvap	72.04	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	7.303		Crippen Method
mvol	328.280	ml/mol	McGowan Method
pc	942.68	kPa	Joback Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	775.38	K	Joback Method
tc	954.93	K	Joback Method
tf	397.28	K	Joback Method
vc	1.274	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.45	J/molxK	775.38	Joback Method
cpg	1053.17	J/molxK	805.30	Joback Method
cpg	1072.83	J/molxK	835.23	Joback Method
cpg	1091.47	J/molxK	865.15	Joback Method
cpg	1109.12	J/molxK	895.08	Joback Method
cpg	1125.83	J/molxK	925.00	Joback Method
cpg	1141.64	J/molxK	954.93	Joback Method
dvisc	0.0017105	Paxs	397.28	Joback Method

dvisc	0.0006024	Paxs	460.30	Joback Method
dvisc	0.0002727	Paxs	523.31	Joback Method
dvisc	0.0001464	Paxs	586.33	Joback Method
dvisc	0.0000887	Paxs	649.35	Joback Method
dvisc	0.0000587	Paxs	712.36	Joback Method
dvisc	0.0000416	Paxs	775.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406064&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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