

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

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

Physical Properties

Property code	Value	Unit	Source
gf	-101.60	kJ/mol	Joback Method
hf	-761.52	kJ/mol	Joback Method
hfus	41.06	kJ/mol	Joback Method
hvap	71.65	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	7.301		Crippen Method
mvol	328.280	ml/mol	McGowan Method
pc	947.33	kPa	Joback Method
rinpol	2077.00		NIST Webbook
rinpol	2077.00		NIST Webbook
tb	774.94	K	Joback Method
tc	955.64	K	Joback Method
tf	382.28	K	Joback Method
vc	1.268	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.89	J/molxK	774.94	Joback Method
cpg	1053.76	J/molxK	805.06	Joback Method
cpg	1073.54	J/molxK	835.17	Joback Method
cpg	1092.27	J/molxK	865.29	Joback Method
cpg	1110.00	J/molxK	895.41	Joback Method
cpg	1126.77	J/molxK	925.53	Joback Method
cpg	1142.63	J/molxK	955.64	Joback Method
dvisc	0.0022274	Paxs	382.28	Joback Method

dvisc	0.0006896	Paxs	447.72	Joback Method
dvisc	0.0002879	Paxs	513.17	Joback Method
dvisc	0.0001465	Paxs	578.61	Joback Method
dvisc	0.0000855	Paxs	644.05	Joback Method
dvisc	0.0000551	Paxs	709.50	Joback Method
dvisc	0.0000383	Paxs	774.94	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=U406263&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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