Hexanoic acid, 3,5,5-trimethyl-, tridec-6-yl ester

Inchi: InChI=1S/C22H44O2/c1-7-9-11-12-14-16-20(15-13-10-8-2)24-21(23)17-19(3)18-22(4,5)6

InchiKey: AUFHVUVLSWCFOE-UHFFFAOYSA-N

Formula: C22H44O2

SMILES: CCCCCCCC(CCCCC)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
mcvol	328.280	ml/mol	McGowan Method
pc	947.33	kPa	Joback Method
rinpol	2056.00		NIST Webbook
rinpol	2056.00		NIST Webbook
tb	774.94	K	Joback Method
tc	955.64	K	Joback Method
tf	382.28	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.89	J/mol×K	774.94	Joback Method
cpg	1126.77	J/mol×K	925.53	Joback Method
cpg	1110.00	J/mol×K	895.41	Joback Method
cpg	1092.27	J/mol×K	865.29	Joback Method
cpg	1073.54	J/mol×K	835.17	Joback Method
cpg	1053.76	J/mol×K	805.06	Joback Method
cpg	1142.63	J/mol×K	955.64	Joback Method
dvisc	0.0000383	Pa×s	774.94	Joback Method

dvisc	0.0000551	Pa×s	709.50	Joback Method
dvisc	0.0000855	Pa×s	644.05	Joback Method
dvisc	0.0001465	Pa×s	578.61	Joback Method
dvisc	0.0002879	Pa×s	513.17	Joback Method
dvisc	0.0006896	Pa×s	447.72	Joback Method
dvisc	0.0022274	Pa×s	382.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406265&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