Hexanoic acid, 3,5,5-trimethyl-, dodec-2-en-1-yl ester

Inchi: InChI=1S/C21H40O2/c1-6-7-8-9-10-11-12-13-14-15-16-23-20(22)17-19(2)18-21(3,4)5/h1

InchiKey: CBQKZGDNXBUUSF-CCEZHUSRSA-N

Formula: C21H40O2

SMILES: CCCCCCCCCC=CCOC(=O)CC(C)CC(C)(C)C

Mol. weight [g/mol]: 324.54

Physical Properties

Property code	Value	Unit	Source
gf	-27.36	kJ/mol	Joback Method
hf	-618.38	kJ/mol	Joback Method
hfus	42.20	kJ/mol	Joback Method
hvap	69.77	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.689		Crippen Method
mcvol	309.890	ml/mol	McGowan Method
pc	1034.57	kPa	Joback Method
rinpol	2138.00		NIST Webbook
rinpol	2138.00		NIST Webbook
tb	756.66	K	Joback Method
tc	937.94	K	Joback Method
tf	380.93	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	947.45	J/mol×K	756.66	Joback Method
cpg	967.34	J/mol×K	786.87	Joback Method
cpg	986.22	J/mol×K	817.09	Joback Method
cpg	1004.14	J/mol×K	847.30	Joback Method
cpg	1021.14	J/mol×K	877.51	Joback Method
cpg	1037.27	J/mol×K	907.73	Joback Method
cpg	1052.58	J/mol×K	937.94	Joback Method
dvisc	0.0018574	Pa×s	380.93	Joback Method

dvisc	0.0006315	Pa×s	443.55	Joback Method
dvisc	0.0002804	Pa×s	506.17	Joback Method
dvisc	0.0001489	Pa×s	568.79	Joback Method
dvisc	0.0000896	Pa×s	631.42	Joback Method
dvisc	0.0000591	Pa×s	694.04	Joback Method
dvisc	0.0000418	Pa×s	756.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406829&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
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