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

Inchi: InChI=1S/C20H38O2/c1-6-7-8-9-10-11-12-13-14-15-22-19(21)16-18(2)17-20(3,4)5/h13-1
InchiKey: VTNXLIHCQGNOCF-BUHFOSPRSA-N
Formula: C20H38O2
SMILES: CCCCCCCCC=CCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 310.51

Physical Properties

Property code	Value	Unit	Source
gf	-35.78	kJ/mol	Joback Method
hf	-597.74	kJ/mol	Joback Method
hfus	39.61	kJ/mol	Joback Method
hvap	67.54	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	6.299		Crippen Method
mcvol	295.800	ml/mol	McGowan Method
pc	1101.54	kPa	Joback Method
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook
tb	733.78	K	Joback Method
tc	914.28	K	Joback Method
tf	369.66	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	887.48	J/mol×K	733.78	Joback Method
cpg	907.07	J/mol×K	763.86	Joback Method
cpg	925.67	J/mol×K	793.95	Joback Method
cpg	943.33	J/mol×K	824.03	Joback Method
cpg	960.09	J/mol×K	854.12	Joback Method
cpg	975.99	J/mol×K	884.20	Joback Method
cpg	991.09	J/mol×K	914.28	Joback Method
dvisc	0.0021217	Pa×s	369.66	Joback Method

dvisc	0.0007245	Pa×s	430.35	Joback Method
dvisc	0.0003227	Pa×s	491.03	Joback Method
dvisc	0.0001717	Pa×s	551.72	Joback Method
dvisc	0.0001035	Pa×s	612.41	Joback Method
dvisc	0.0000684	Pa×s	673.09	Joback Method
dvisc	0.0000484	Pa×s	733.78	Joback Method

Sources

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=U406932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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