Dimethylmalonic acid, 1-phenyl-2-(cyclohex-2-enyl)ethyl tridecyl ester

Inchi: InChI=1S/C32H50O4/c1-4-5-6-7-8-9-10-11-12-13-20-25-35-30(33)32(2,3)31(34)36-29(28
InchiKey: NTAGOVGMGYPSMP-UHFFFAOYSA-N
Formula: C32H50O4
SMILES: CCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 498.74

Physical Properties

Property code	Value	Unit	Source
gf	-82.06	kJ/mol	Joback Method
hf	-858.81	kJ/mol	Joback Method
hfus	60.37	kJ/mol	Joback Method
hvap	106.45	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	8.898		Crippen Method
mcvol	437.700	ml/mol	McGowan Method
pc	772.03	kPa	Joback Method
rinpol	3294.00		NIST Webbook
rinpol	3294.00		NIST Webbook
tb	1125.86	K	Joback Method
tc	1382.96	K	Joback Method
tf	616.70	K	Joback Method
vc	1.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1584.81	J/mol×K	1125.86	Joback Method
cpg	1601.89	J/mol×K	1168.71	Joback Method
cpg	1617.14	J/mol×K	1211.56	Joback Method
cpg	1630.75	J/mol×K	1254.41	Joback Method
cpg	1642.86	J/mol×K	1297.26	Joback Method
cpg	1653.66	J/mol×K	1340.11	Joback Method
cpg	1663.30	J/mol×K	1382.96	Joback Method
dvisc	0.0001630	Pa×s	616.70	Joback Method

dvisc	0.0000688	Pa×s	701.56	Joback Method
dvisc	0.0000350	Pa×s	786.42	Joback Method
dvisc	0.0000203	Pa×s	871.28	Joback Method
dvisc	0.0000129	Pa×s	956.14	Joback Method
dvisc	0.0000089	Pa×s	1041.00	Joback Method
dvisc	0.0000065	Pa×s	1125.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361879&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