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

Inchi: InChI=1S/C30H46O4/c1-4-5-6-7-8-9-10-11-18-23-33-28(31)30(2,3)29(32)34-27(26-21-16
InchiKey: NTXLBALGKHQCGC-UHFFFAOYSA-N
Formula: C30H46O4
SMILES: CCCCCCCCCCCOC(=O)C(C)(C)C(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 470.68

Physical Properties

Property code	Value	Unit	Source
gf	-98.90	kJ/mol	Joback Method
hf	-817.53	kJ/mol	Joback Method
hfus	55.19	kJ/mol	Joback Method
hvap	102.00	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	8.117		Crippen Method
mcvol	409.520	ml/mol	McGowan Method
pc	861.50	kPa	Joback Method
rinpol	3090.00		NIST Webbook
tb	1080.10	K	Joback Method
tc	1322.68	K	Joback Method
tf	594.16	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1457.91	J/mol×K	1080.10	Joback Method
cpg	1474.59	J/mol×K	1120.53	Joback Method
cpg	1489.57	J/mol×K	1160.96	Joback Method
cpg	1503.00	J/mol×K	1201.39	Joback Method
cpg	1514.99	J/mol×K	1241.82	Joback Method
cpg	1525.68	J/mol×K	1282.25	Joback Method
cpg	1535.20	J/mol×K	1322.68	Joback Method
dvisc	0.0002187	Pa×s	594.16	Joback Method
dvisc	0.0000935	Pa×s	675.15	Joback Method

dvisc	0.0000479	Pa×s	756.14	Joback Method
dvisc	0.0000279	Pa×s	837.13	Joback Method
dvisc	0.0000179	Pa×s	918.12	Joback Method
dvisc	0.0000124	Pa×s	999.11	Joback Method
dvisc	0.0000090	Pa×s	1080.10	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361877&Units=SI

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