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

Inchi: InChI=1S/C29H44O4/c1-4-5-6-7-8-9-10-17-22-32-27(30)29(2,3)28(31)33-26(25-20-15-12
InchiKey: RFCTVWVKFJHBIY-UHFFFAOYSA-N
Formula: C29H44O4
SMILES: CCCCCCCCCCOC(=O)C(C)(C)C(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 456.66

Physical Properties

Property code	Value	Unit	Source
gf	-107.32	kJ/mol	Joback Method
hf	-796.89	kJ/mol	Joback Method
hfus	52.60	kJ/mol	Joback Method
hvap	99.77	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.727		Crippen Method
mcvol	395.430	ml/mol	McGowan Method
pc	912.18	kPa	Joback Method
rinpol	2994.00		NIST Webbook
tb	1057.22	K	Joback Method
tc	1294.37	K	Joback Method
tf	582.89	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.88	J/mol×K	1057.22	Joback Method
cpg	1411.44	J/mol×K	1096.74	Joback Method
cpg	1426.36	J/mol×K	1136.27	Joback Method
cpg	1439.75	J/mol×K	1175.79	Joback Method
cpg	1451.73	J/mol×K	1215.32	Joback Method
cpg	1462.41	J/mol×K	1254.84	Joback Method
cpg	1471.93	J/mol×K	1294.37	Joback Method
dvisc	0.0002527	Pa×s	582.89	Joback Method
dvisc	0.0001087	Pa×s	661.94	Joback Method

dvisc	0.0000560	Pa×s	741.00	Joback Method
dvisc	0.0000328	Pa×s	820.06	Joback Method
dvisc	0.0000211	Pa×s	899.11	Joback Method
dvisc	0.0000145	Pa×s	978.16	Joback Method
dvisc	0.0000106	Pa×s	1057.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361876&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

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