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

Inchi: InChI=1S/C31H48O4/c1-4-5-6-7-8-9-10-11-12-19-24-34-29(32)31(2,3)30(33)35-28(27-22
InchiKey: RBFFBCDOGUOTEA-UHFFFAOYSA-N
Formula: C31H48O4
SMILES: CCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 484.71

Physical Properties

Property code	Value	Unit	Source
gf	-90.48	kJ/mol	Joback Method
hf	-838.17	kJ/mol	Joback Method
hfus	57.78	kJ/mol	Joback Method
hvap	104.22	kJ/mol	Joback Method
log10ws	-9.35		Crippen Method
logp	8.508		Crippen Method
mcvol	423.610	ml/mol	McGowan Method
pc	814.93	kPa	Joback Method
rinpol	3193.00		NIST Webbook
tb	1102.98	K	Joback Method
tc	1352.18	K	Joback Method
tf	605.43	K	Joback Method
vc	1.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.22	J/mol×K	1102.98	Joback Method
cpg	1589.42	J/mol×K	1310.65	Joback Method
cpg	1578.70	J/mol×K	1269.11	Joback Method
cpg	1566.67	J/mol×K	1227.58	Joback Method
cpg	1553.17	J/mol×K	1186.05	Joback Method
cpg	1538.07	J/mol×K	1144.51	Joback Method
cpg	1598.98	J/mol×K	1352.18	Joback Method
dvisc	0.0000076	Pa×s	1102.98	Joback Method
dvisc	0.0000105	Pa×s	1020.06	Joback Method

dvisc	0.0000152	Pa×s	937.13	Joback Method
dvisc	0.0000238	Pa×s	854.21	Joback Method
dvisc	0.0000409	Pa×s	771.28	Joback Method
dvisc	0.0000802	Pa×s	688.36	Joback Method
dvisc	0.0001890	Pa×s	605.43	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=U361878&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