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

Inchi: InChI=1S/C28H42O4/c1-4-5-6-7-8-9-16-21-31-26(29)28(2,3)27(30)32-25(24-19-14-11-15
InchiKey: RCLYKKHXFZUHCL-UHFFFAOYSA-N
Formula: C28H42O4
SMILES: CCCCCCCCCOC(=O)C(C)(C)C(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 442.63

Physical Properties

Property code	Value	Unit	Source
gf	-115.74	kJ/mol	Joback Method
hf	-776.25	kJ/mol	Joback Method
hfus	50.01	kJ/mol	Joback Method
hvap	97.55	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	7.337		Crippen Method
mcvol	381.340	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
rinpol	2873.00		NIST Webbook
rinpol	2873.00		NIST Webbook
tb	1034.34	K	Joback Method
tc	1267.18	K	Joback Method
tf	571.62	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.18	J/mol×K	1034.34	Joback Method
cpg	1399.63	J/mol×K	1228.37	Joback Method
cpg	1388.92	J/mol×K	1189.57	Joback Method
cpg	1376.93	J/mol×K	1150.76	Joback Method
cpg	1363.54	J/mol×K	1111.95	Joback Method
cpg	1348.66	J/mol×K	1073.15	Joback Method
cpg	1409.17	J/mol×K	1267.18	Joback Method
dvisc	0.0000125	Pa×s	1034.34	Joback Method

dvisc	0.0000171	Pa×s	957.22	Joback Method
dvisc	0.0000247	Pa×s	880.10	Joback Method
dvisc	0.0000383	Pa×s	802.98	Joback Method
dvisc	0.0000653	Pa×s	725.86	Joback Method
dvisc	0.0001262	Pa×s	648.74	Joback Method
dvisc	0.0002913	Pa×s	571.62	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=U361875&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