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

Inchi: InChI=1S/C27H40O4/c1-4-5-6-7-8-15-20-30-25(28)27(2,3)26(29)31-24(23-18-13-10-14-1

InchiKey: XFBAGDLWFUZFGA-UHFFFAOYSA-N

Formula: C27H40O4

SMILES: CCCCCCCCOC(=O)C(C)(C)C(=O)OC(CC1C=CCCC1)c1ccccc1

Mol. weight [g/mol]: 428.60

Physical Properties

Property code	Value	Unit	Source
gf	-124.16	kJ/mol	Joback Method
hf	-755.61	kJ/mol	Joback Method
hfus	47.42	kJ/mol	Joback Method
hvap	95.32	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.947		Crippen Method
mcvol	367.250	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	2769.00		NIST Webbook
tb	1011.46	K	Joback Method
tc	1241.04	K	Joback Method
tf	560.35	K	Joback Method
vc	1.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1269.83	J/mol×K	1011.46	Joback Method
cpg	1286.28	J/mol×K	1049.72	Joback Method
cpg	1301.16	J/mol×K	1087.99	Joback Method
cpg	1314.56	J/mol×K	1126.25	Joback Method
cpg	1326.59	J/mol×K	1164.51	Joback Method
cpg	1337.35	J/mol×K	1202.78	Joback Method
cpg	1346.92	J/mol×K	1241.04	Joback Method
dvisc	0.0003352	Pa×s	560.35	Joback Method
dvisc	0.0001462	Pa×s	635.53	Joback Method

dvisc	0.0000760	Pa×s	710.72	Joback Method
dvisc	0.0000448	Pa×s	785.90	Joback Method
dvisc	0.0000290	Pa×s	861.09	Joback Method
dvisc	0.0000201	Pa×s	936.27	Joback Method
dvisc	0.0000147	Pa×s	1011.46	Joback Method

Sources

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=U361874&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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