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

Inchi: InChI=1S/C26H38O4/c1-4-5-6-7-14-19-29-24(27)26(2,3)25(28)30-23(22-17-12-9-13-18-2
InchiKey: UKANIDFILJAQNW-UHFFFAOYSA-N
Formula: C26H38O4
SMILES: CCCCCCCOC(=O)C(C)(C)C(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 414.58

Physical Properties

Property code	Value	Unit	Source
gf	-132.58	kJ/mol	Joback Method
hf	-734.97	kJ/mol	Joback Method
hfus	44.83	kJ/mol	Joback Method
hvap	93.09	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.557		Crippen Method
mcvol	353.160	ml/mol	McGowan Method
pc	1094.27	kPa	Joback Method
rinpol	2677.00		NIST Webbook
tb	988.58	K	Joback Method
tc	1215.89	K	Joback Method
tf	549.08	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1207.86	J/mol×K	988.58	Joback Method
cpg	1224.31	J/mol×K	1026.47	Joback Method
cpg	1239.22	J/mol×K	1064.35	Joback Method
cpg	1252.67	J/mol×K	1102.24	Joback Method
cpg	1264.75	J/mol×K	1140.12	Joback Method
cpg	1275.56	J/mol×K	1178.01	Joback Method
cpg	1285.19	J/mol×K	1215.89	Joback Method
dvisc	0.0003849	Pa×s	549.08	Joback Method
dvisc	0.0001692	Pa×s	622.33	Joback Method

dvisc	0.0000884	Pa×s	695.58	Joback Method
dvisc	0.0000523	Pa×s	768.83	Joback Method
dvisc	0.0000339	Pa×s	842.08	Joback Method
dvisc	0.0000235	Pa×s	915.33	Joback Method
dvisc	0.0000172	Pa×s	988.58	Joback Method

Sources

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=U361873&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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