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

Inchi: InChI=1S/C25H36O4/c1-4-5-6-13-18-28-23(26)25(2,3)24(27)29-22(21-16-11-8-12-17-21)
InchiKey: NBSIYRZZJFENLN-UHFFFAOYSA-N
Formula: C25H36O4
SMILES: CCCCCCOC(=O)C(C)(C)C(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-141.00	kJ/mol	Joback Method
hf	-714.33	kJ/mol	Joback Method
hfus	42.24	kJ/mol	Joback Method
hvap	90.87	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.167		Crippen Method
mcvol	339.070	ml/mol	McGowan Method
pc	1167.22	kPa	Joback Method
rinpol	2586.00		NIST Webbook
rinpol	2586.00		NIST Webbook
tb	965.70	K	Joback Method
tc	1191.67	K	Joback Method
tf	537.81	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.31	J/mol×K	965.70	Joback Method
cpg	1214.29	J/mol×K	1154.01	Joback Method
cpg	1203.42	J/mol×K	1116.35	Joback Method
cpg	1191.27	J/mol×K	1078.69	Joback Method
cpg	1177.76	J/mol×K	1041.02	Joback Method
cpg	1162.80	J/mol×K	1003.36	Joback Method
cpg	1223.98	J/mol×K	1191.67	Joback Method
dvisc	0.0000202	Pa×s	965.70	Joback Method

dvisc	0.0000275	Pa×s	894.38	Joback Method
dvisc	0.0000396	Pa×s	823.07	Joback Method
dvisc	0.0000609	Pa×s	751.75	Joback Method
dvisc	0.0001026	Pa×s	680.44	Joback Method
dvisc	0.0001953	Pa×s	609.12	Joback Method
dvisc	0.0004409	Pa×s	537.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361872&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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