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

Inchi: InChI=1S/C22H30O4/c1-4-15-25-20(23)22(2,3)21(24)26-19(18-13-9-6-10-14-18)16-17-1
InchiKey: QEDJNZDPFQOXKW-UHFFFAOYSA-N
Formula: C22H30O4
SMILES: CCCOC(=O)C(C)(C)C(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 358.47

Physical Properties

Property code	Value	Unit	Source
gf	-166.26	kJ/mol	Joback Method
hf	-652.41	kJ/mol	Joback Method
hfus	34.47	kJ/mol	Joback Method
hvap	84.19	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.997		Crippen Method
mcvol	296.800	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	2315.00		NIST Webbook
tb	897.06	K	Joback Method
tc	1124.04	K	Joback Method
tf	504.00	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.66	J/mol×K	897.06	Joback Method
cpg	981.38	J/mol×K	934.89	Joback Method
cpg	996.57	J/mol×K	972.72	Joback Method
cpg	1010.32	J/mol×K	1010.55	Joback Method
cpg	1022.69	J/mol×K	1048.38	Joback Method
cpg	1033.76	J/mol×K	1086.21	Joback Method
cpg	1043.62	J/mol×K	1124.04	Joback Method
dvisc	0.0006527	Pa×s	504.00	Joback Method
dvisc	0.0002964	Pa×s	569.51	Joback Method

dvisc	0.0001584	Pa×s	635.02	Joback Method
dvisc	0.0000952	Pa×s	700.53	Joback Method
dvisc	0.0000624	Pa×s	766.04	Joback Method
dvisc	0.0000437	Pa×s	831.55	Joback Method
dvisc	0.0000323	Pa×s	897.06	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=U361869&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