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

Inchi: InChI=1S/C33H40O4/c1-33(2,31(34)36-29(27-19-11-5-12-20-27)23-25-15-7-3-8-16-25)3

InchiKey: CBHUXZAKRXLXKL-UHFFFAOYSA-N

Formula: C33H40O4

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

Mol. weight [g/mol]: 500.67

Physical Properties

Property code	Value	Unit	Source
gf	90.74	kJ/mol	Joback Method
hf	-536.10	kJ/mol	Joback Method
hfus	46.54	kJ/mol	Joback Method
hvap	111.29	kJ/mol	Joback Method
log10ws	-9.26		Crippen Method
logp	8.074		Crippen Method
mcvol	412.870	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	3400.00		NIST Webbook
rinpol	3400.00		NIST Webbook
tb	1193.69	K	Joback Method
tc	1464.22	K	Joback Method
tf	647.53	K	Joback Method
vc	1.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1484.22	J/mol×K	1193.69	Joback Method
cpg	1496.09	J/mol×K	1238.78	Joback Method
cpg	1506.36	J/mol×K	1283.87	Joback Method
cpg	1515.28	J/mol×K	1328.96	Joback Method
cpg	1523.04	J/mol×K	1374.05	Joback Method
cpg	1529.89	J/mol×K	1419.13	Joback Method
cpg	1536.04	J/mol×K	1464.22	Joback Method
dvisc	0.0001495	Pa×s	647.53	Joback Method

dvisc	0.0000624	Pa×s	738.56	Joback Method
dvisc	0.0000315	Pa×s	829.58	Joback Method
dvisc	0.0000182	Pa×s	920.61	Joback Method
dvisc	0.0000116	Pa×s	1011.64	Joback Method
dvisc	0.0000080	Pa×s	1102.66	Joback Method
dvisc	0.0000058	Pa×s	1193.69	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=U361880&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