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

Inchi: InChI=1S/C23H32O4/c1-17(2)16-26-21(24)23(3,4)22(25)27-20(19-13-9-6-10-14-19)15-18

InchiKey: HIOIJAZHDPSNBD-UHFFFAOYSA-N

Formula: C23H32O4

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

Mol. weight [g/mol]: 372.50

Physical Properties

Property code	Value	Unit	Source
gf	-160.28	kJ/mol	Joback Method
hf	-678.33	kJ/mol	Joback Method
hfus	33.54	kJ/mol	Joback Method
hvap	86.03	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.243		Crippen Method
mcvol	310.890	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	2359.00		NIST Webbook
tb	919.50	K	Joback Method
tc	1147.79	K	Joback Method
tf	500.27	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1025.13	J/mol×K	919.50	Joback Method
cpg	1094.08	J/mol×K	1109.74	Joback Method
cpg	1083.10	J/mol×K	1071.69	Joback Method
cpg	1070.80	J/mol×K	1033.64	Joback Method
cpg	1057.09	J/mol×K	995.60	Joback Method
cpg	1041.89	J/mol×K	957.55	Joback Method
cpg	1103.81	J/mol×K	1147.79	Joback Method
dvisc	0.0000253	Pa×s	919.50	Joback Method
dvisc	0.0000348	Pa×s	849.63	Joback Method

dvisc	0.0000508	Pa×s	779.76	Joback Method
dvisc	0.0000800	Pa×s	709.88	Joback Method
dvisc	0.0001390	Pa×s	640.01	Joback Method
dvisc	0.0002764	Pa×s	570.14	Joback Method
dvisc	0.0006661	Pa×s	500.27	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=U361870&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