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

Inchi: InChI=1S/C23H32O4/c1-4-5-16-26-21(24)23(2,3)22(25)27-20(19-14-10-7-11-15-19)17-18

InchiKey: YTIJBNMRBBRZJG-UHFFFAOYSA-N

Formula: C23H32O4

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

Mol. weight [g/mol]: 372.50

Physical Properties

Property code	Value	Unit	Source
gf	-157.84	kJ/mol	Joback Method
hf	-673.05	kJ/mol	Joback Method
hfus	37.06	kJ/mol	Joback Method
hvap	86.42	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.387		Crippen Method
mcvol	310.890	ml/mol	McGowan Method
pc	1336.86	kPa	Joback Method
rinpol	2403.00		NIST Webbook
tb	919.94	K	Joback Method
tc	1145.80	K	Joback Method
tf	515.27	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.67	J/mol×K	919.94	Joback Method
cpg	1093.38	J/mol×K	1108.15	Joback Method
cpg	1082.36	J/mol×K	1070.51	Joback Method
cpg	1070.07	J/mol×K	1032.87	Joback Method
cpg	1056.40	J/mol×K	995.23	Joback Method
cpg	1041.30	J/mol×K	957.58	Joback Method
cpg	1103.18	J/mol×K	1145.80	Joback Method
dvisc	0.0000277	Pa×s	919.94	Joback Method
dvisc	0.0000375	Pa×s	852.50	Joback Method

dvisc	0.0000537	Pa×s	785.05	Joback Method
dvisc	0.0000822	Pa×s	717.61	Joback Method
dvisc	0.0001373	Pa×s	650.16	Joback Method
dvisc	0.0002585	Pa×s	582.72	Joback Method
dvisc	0.0005743	Pa×s	515.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361871&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