Dimethylmalonic acid, butyl 4-(4-methoxyphenyl)cyclohexyl ester

Inchi: InChI=1S/C22H32O5/c1-5-6-15-26-20(23)22(2,3)21(24)27-19-13-9-17(10-14-19)16-7-11-
InchiKey: SNADJYBKZGAIDL-UHFFFAOYSA-N
Formula: C22H32O5
SMILES: CCCCOC(=O)C(C)(C)C(=O)OC1CCC(c2ccc(OC)cc2)CC1
Mol. weight [g/mol]: 376.49

Physical Properties

Property code	Value	Unit	Source
gf	-316.12	kJ/mol	Joback Method
hf	-868.94	kJ/mol	Joback Method
hfus	38.64	kJ/mol	Joback Method
hvap	87.05	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.634		Crippen Method
mcvol	306.970	ml/mol	McGowan Method
pc	1324.24	kPa	Joback Method
rinpol	2804.00		NIST Webbook
tb	921.07	K	Joback Method
tc	1144.76	K	Joback Method
tf	548.75	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1026.59	J/mol×K	921.07	Joback Method
cpg	1092.41	J/mol×K	1107.48	Joback Method
cpg	1082.50	J/mol×K	1070.20	Joback Method
cpg	1071.01	J/mol×K	1032.92	Joback Method
cpg	1057.88	J/mol×K	995.63	Joback Method
cpg	1043.09	J/mol×K	958.35	Joback Method
cpg	1100.76	J/mol×K	1144.76	Joback Method
dvisc	0.0000322	Pa×s	921.07	Joback Method
dvisc	0.0000419	Pa×s	859.02	Joback Method

dvisc	0.0000567	Pa×s	796.96	Joback Method
dvisc	0.0000807	Pa×s	734.91	Joback Method
dvisc	0.0001228	Pa×s	672.86	Joback Method
dvisc	0.0002033	Pa×s	610.80	Joback Method
dvisc	0.0003772	Pa×s	548.75	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=U363915&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

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