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

Inchi: InChI=1S/C24H36O5/c1-17(2)7-6-16-28-22(25)24(3,4)23(26)29-21-14-10-19(11-15-21)18

InchiKey: UTKLXWSDVDWJOA-UHFFFAOYSA-N

Formula: C24H36O5

SMILES: COc1ccc(C2CCC(OC(=O)C(C)(C)C(=O)OCCCC(C)C)CC2)cc1

Mol. weight [g/mol]: 404.54

Physical Properties

Property code	Value	Unit	Source
gf	-301.72	kJ/mol	Joback Method
hf	-915.50	kJ/mol	Joback Method
hfus	40.30	kJ/mol	Joback Method
hvap	91.11	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.270		Crippen Method
mcvol	335.150	ml/mol	McGowan Method
pc	1163.25	kPa	Joback Method
rinpol	2978.00		NIST Webbook
rinpol	2978.00		NIST Webbook
tb	966.39	K	Joback Method
tc	1192.48	K	Joback Method
tf	556.29	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1148.69	J/mol×K	966.39	Joback Method
cpg	1164.88	J/mol×K	1004.07	Joback Method
cpg	1179.27	J/mol×K	1041.75	Joback Method
cpg	1191.89	J/mol×K	1079.43	Joback Method
cpg	1202.79	J/mol×K	1117.11	Joback Method
cpg	1212.02	J/mol×K	1154.79	Joback Method
cpg	1219.62	J/mol×K	1192.48	Joback Method
dvisc	0.0003292	Pa×s	556.29	Joback Method

dvisc	0.0001632	Pa×s	624.64	Joback Method
dvisc	0.0000930	Pa×s	692.99	Joback Method
dvisc	0.0000586	Pa×s	761.34	Joback Method
dvisc	0.0000398	Pa×s	829.69	Joback Method
dvisc	0.0000287	Pa×s	898.04	Joback Method
dvisc	0.0000217	Pa×s	966.39	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=U363917&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