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

Inchi: InChI=1S/C24H36O5/c1-5-6-7-8-17-28-22(25)24(2,3)23(26)29-21-15-11-19(12-16-21)18-
InchiKey: GQNYYGJLAJXPJJ-UHFFFAOYSA-N
Formula: C24H36O5
SMILES: CCCCCCOC(=O)C(C)(C)C(=O)OC1CCC(c2ccc(OC)cc2)CC1
Mol. weight [g/mol]: 404.54

Physical Properties

Property code	Value	Unit	Source
gf	-299.28	kJ/mol	Joback Method
hf	-910.22	kJ/mol	Joback Method
hfus	43.82	kJ/mol	Joback Method
hvap	91.50	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.414		Crippen Method
mcvol	335.150	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinpol	3014.00		NIST Webbook
rinpol	3014.00		NIST Webbook
tb	966.83	K	Joback Method
tc	1191.38	K	Joback Method
tf	571.29	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1148.29	J/mol×K	966.83	Joback Method
cpg	1211.71	J/mol×K	1153.96	Joback Method
cpg	1202.39	J/mol×K	1116.53	Joback Method
cpg	1191.44	J/mol×K	1079.11	Joback Method
cpg	1178.80	J/mol×K	1041.68	Joback Method
cpg	1164.43	J/mol×K	1004.26	Joback Method
cpg	1219.44	J/mol×K	1191.38	Joback Method
dvisc	0.0000238	Pa×s	966.83	Joback Method

dvisc	0.0000311	Pa×s	900.91	Joback Method
dvisc	0.0000423	Pa×s	834.98	Joback Method
dvisc	0.0000608	Pa×s	769.06	Joback Method
dvisc	0.0000935	Pa×s	703.14	Joback Method
dvisc	0.0001572	Pa×s	637.21	Joback Method
dvisc	0.0002977	Pa×s	571.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363918&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

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