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

Inchi: InChI=1S/C25H38O5/c1-5-6-7-8-9-18-29-23(26)25(2,3)24(27)30-22-16-12-20(13-17-22)1

InchiKey: UNQHJXAURLXHEY-UHFFFAOYSA-N

Formula: C25H38O5

SMILES: CCCCCCCOC(=O)C(C)(C)C(=O)OC1CCC(c2ccc(OC)cc2)CC1

Mol. weight [g/mol]: 418.57

Physical Properties

Property code	Value	Unit	Source
gf	-290.86	kJ/mol	Joback Method
hf	-930.86	kJ/mol	Joback Method
hfus	46.41	kJ/mol	Joback Method
hvap	93.73	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.804		Crippen Method
mcvol	349.240	ml/mol	McGowan Method
pc	1084.92	kPa	Joback Method
rinpol	3111.00		NIST Webbook
tb	989.71	K	Joback Method
tc	1215.99	K	Joback Method
tf	582.56	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1209.73	J/mol×K	989.71	Joback Method
cpg	1271.88	J/mol×K	1178.28	Joback Method
cpg	1262.89	J/mol×K	1140.56	Joback Method
cpg	1252.24	J/mol×K	1102.85	Joback Method
cpg	1239.86	J/mol×K	1065.14	Joback Method
cpg	1225.71	J/mol×K	1027.42	Joback Method
cpg	1279.24	J/mol×K	1215.99	Joback Method
dvisc	0.0000204	Pa×s	989.71	Joback Method
dvisc	0.0000267	Pa×s	921.85	Joback Method

dvisc	0.0000365	Pa×s	853.99	Joback Method
dvisc	0.0000526	Pa×s	786.13	Joback Method
dvisc	0.0000813	Pa×s	718.28	Joback Method
dvisc	0.0001376	Pa×s	650.42	Joback Method
dvisc	0.0002633	Pa×s	582.56	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=U363919&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