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

Inchi: InChI=1S/C23H34O5/c1-5-6-7-16-27-21(24)23(2,3)22(25)28-20-14-10-18(11-15-20)17-8-

InchiKey: RONFBDJYLKNLSM-UHFFFAOYSA-N

Formula: C23H34O5

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

Mol. weight [g/mol]: 390.51

Physical Properties

Property code	Value	Unit	Source
gf	-307.70	kJ/mol	Joback Method
hf	-889.58	kJ/mol	Joback Method
hfus	41.23	kJ/mol	Joback Method
hvap	89.28	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.024		Crippen Method
mcvol	321.060	ml/mol	McGowan Method
pc	1236.35	kPa	Joback Method
rinpol	2910.00		NIST Webbook
tb	943.95	K	Joback Method
tc	1167.65	K	Joback Method
tf	560.02	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.22	J/mol×K	943.95	Joback Method
cpg	1103.54	J/mol×K	981.23	Joback Method
cpg	1118.12	J/mol×K	1018.52	Joback Method
cpg	1131.01	J/mol×K	1055.80	Joback Method
cpg	1142.25	J/mol×K	1093.09	Joback Method
cpg	1151.87	J/mol×K	1130.37	Joback Method
cpg	1159.93	J/mol×K	1167.65	Joback Method
dvisc	0.0003356	Pa×s	560.02	Joback Method
dvisc	0.0001790	Pa×s	624.01	Joback Method

dvisc	0.0001073	Pa×s	688.00	Joback Method
dvisc	0.0000702	Pa×s	751.98	Joback Method
dvisc	0.0000490	Pa×s	815.97	Joback Method
dvisc	0.0000361	Pa×s	879.96	Joback Method
dvisc	0.0000277	Pa×s	943.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363916&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