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

Inchi: InChI=1S/C26H40O5/c1-5-6-7-8-9-10-19-30-24(27)26(2,3)25(28)31-23-17-13-21(14-18-2

InchiKey: KPJMGEGBSKAEQQ-UHFFFAOYSA-N

Formula: C26H40O5

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

Mol. weight [g/mol]: 432.59

Physical Properties

Property code	Value	Unit	Source
gf	-282.44	kJ/mol	Joback Method
hf	-951.50	kJ/mol	Joback Method
hfus	49.00	kJ/mol	Joback Method
hvap	95.95	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	6.194		Crippen Method
mcvol	363.330	ml/mol	McGowan Method
pc	1019.43	kPa	Joback Method
rinpol	3207.00		NIST Webbook
tb	1012.59	K	Joback Method
tc	1241.55	K	Joback Method
tf	593.83	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1271.51	J/mol×K	1012.59	Joback Method
cpg	1332.33	J/mol×K	1203.39	Joback Method
cpg	1323.71	J/mol×K	1165.23	Joback Method
cpg	1313.37	J/mol×K	1127.07	Joback Method
cpg	1301.26	J/mol×K	1088.91	Joback Method
cpg	1287.33	J/mol×K	1050.75	Joback Method
cpg	1339.29	J/mol×K	1241.55	Joback Method
dvisc	0.0000175	Pa×s	1012.59	Joback Method
dvisc	0.0000229	Pa×s	942.80	Joback Method

dvisc	0.0000314	Pa×s	873.00	Joback Method
dvisc	0.0000454	Pa×s	803.21	Joback Method
dvisc	0.0000706	Pa×s	733.42	Joback Method
dvisc	0.0001203	Pa×s	663.62	Joback Method
dvisc	0.0002323	Pa×s	593.83	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363920&Units=SI

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