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

Inchi: InChI=1S/C18H23ClO4/c1-18(2,16(19)20)17(21)23-15-10-6-13(7-11-15)12-4-8-14(22-3)9

InchiKey: BGQWDRVFTCSLSY-UHFFFAOYSA-N

Formula: C18H23ClO4

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

Mol. weight [g/mol]: 338.83

Physical Properties

Property code	Value	Unit	Source
gf	-256.73	kJ/mol	Joback Method
hf	-669.90	kJ/mol	Joback Method
hfus	31.29	kJ/mol	Joback Method
hvap	80.12	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.056		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinpol	2576.00		NIST Webbook
rinpol	2576.00		NIST Webbook
tb	844.56	K	Joback Method
tc	1080.54	K	Joback Method
tf	511.36	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.67	J/mol×K	844.56	Joback Method
cpg	853.67	J/mol×K	1041.21	Joback Method
cpg	843.43	J/mol×K	1001.88	Joback Method
cpg	831.77	J/mol×K	962.55	Joback Method
cpg	818.62	J/mol×K	923.22	Joback Method
cpg	803.94	J/mol×K	883.89	Joback Method
cpg	862.53	J/mol×K	1080.54	Joback Method
dvisc	0.0000664	Pa×s	844.56	Joback Method

dvisc	0.0000854	Pa×s	789.03	Joback Method
dvisc	0.0001140	Pa×s	733.49	Joback Method
dvisc	0.0001596	Pa×s	677.96	Joback Method
dvisc	0.0002372	Pa×s	622.43	Joback Method
dvisc	0.0003811	Pa×s	566.89	Joback Method
dvisc	0.0006787	Pa×s	511.36	Joback Method

Sources

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=U363925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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