Dimethylmalonic acid, 2,3-dichlorophenyl ethyl ester

Inchi: InChI=1S/C13H14Cl2O4/c1-4-18-11(16)13(2,3)12(17)19-9-7-5-6-8(14)10(9)15/h5-7H,4H

InchiKey: MZKUYRNCZCKCIR-UHFFFAOYSA-N

Formula: C13H14Cl2O4

SMILES: CCOC(=O)C(C)(C)C(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 305.15

Physical Properties

Property code	Value	Unit	Source
gf	-337.13	kJ/mol	Joback Method
hf	-627.89	kJ/mol	Joback Method
hfus	29.24	kJ/mol	Joback Method
hvap	73.92	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.488		Crippen Method
mcvol	209.630	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1912.00		NIST Webbook
tb	757.69	K	Joback Method
tc	984.10	K	Joback Method
tf	494.31	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.95	J/mol×K	757.69	Joback Method
cpg	549.88	J/mol×K	795.42	Joback Method
cpg	560.86	J/mol×K	833.16	Joback Method
cpg	570.89	J/mol×K	870.89	Joback Method
cpg	580.00	J/mol×K	908.63	Joback Method
cpg	588.23	J/mol×K	946.36	Joback Method
cpg	595.60	J/mol×K	984.10	Joback Method
dvisc	0.0006326	Pa×s	494.31	Joback Method
dvisc	0.0003995	Pa×s	538.21	Joback Method

dvisc	0.0002704	Pa×s	582.10	Joback Method
dvisc	0.0001933	Pa×s	626.00	Joback Method
dvisc	0.0001444	Pa×s	669.90	Joback Method
dvisc	0.0001119	Pa×s	713.79	Joback Method
dvisc	0.0000892	Pa×s	757.69	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=U363619&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