Dimethylmalonic acid, 2,5-dichlorophenyl ethyl ester

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

InchiKey: PCRJTCKWWJXKBD-UHFFFAOYSA-N

Formula: C13H14Cl2O4

SMILES: CCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl

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	1863.00		NIST Webbook
rinpol	1863.00		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

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=U363677&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