Dimethylmalonic acid, di(4-chlorophenyl) ester

Inchi: InChI=1S/C17H14Cl2O4/c1-17(2,15(20)22-13-7-3-11(18)4-8-13)16(21)23-14-9-5-12(19)6
InchiKey: VZPKMICWFKFYHC-UHFFFAOYSA-N
Formula: C17H14Cl2O4
SMILES: CC(C)(C(=O)Oc1ccc(Cl)cc1)C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 353.20

Physical Properties

Property code	Value	Unit	Source
gf	-191.04	kJ/mol	Joback Method
hf	-473.92	kJ/mol	Joback Method
hfus	33.64	kJ/mol	Joback Method
hvap	85.10	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.531		Crippen Method
mcvol	242.230	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	2425.00		NIST Webbook
tb	875.89	K	Joback Method
tc	1124.24	K	Joback Method
tf	565.81	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.56	J/mol×K	875.89	Joback Method
cpg	700.56	J/mol×K	1082.85	Joback Method
cpg	693.94	J/mol×K	1041.46	Joback Method
cpg	686.30	J/mol×K	1000.07	Joback Method
cpg	677.57	J/mol×K	958.67	Joback Method
cpg	667.68	J/mol×K	917.28	Joback Method
cpg	706.21	J/mol×K	1124.24	Joback Method
dvisc	0.0000509	Pa×s	875.89	Joback Method
dvisc	0.0000640	Pa×s	824.21	Joback Method

dvisc	0.0000829	Pa×s	772.53	Joback Method
dvisc	0.0001115	Pa×s	720.85	Joback Method
dvisc	0.0001570	Pa×s	669.17	Joback Method
dvisc	0.0002342	Pa×s	617.49	Joback Method
dvisc	0.0003757	Pa×s	565.81	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=U361987&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