Dimethylmalonic acid, di(2,3-dichlorophenyl) ester

Inchi: InChI=1S/C17H12Cl4O4/c1-17(2,15(22)24-11-7-3-5-9(18)13(11)20)16(23)25-12-8-4-6-10
InchiKey: GPXRDTIKSOTOEJ-UHFFFAOYSA-N
Formula: C17H12Cl4O4
SMILES: CC(C)(C(=O)Oc1cccc(Cl)c1Cl)C(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 422.09

Physical Properties

Property code	Value	Unit	Source
gf	-234.16	kJ/mol	Joback Method
hf	-528.34	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	95.19	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.837		Crippen Method
mcvol	266.710	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	960.71	K	Joback Method
tc	1214.73	K	Joback Method
tf	650.69	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.04	J/mol×K	960.71	Joback Method
cpg	697.31	J/mol×K	1003.05	Joback Method
cpg	704.42	J/mol×K	1045.38	Joback Method
cpg	710.44	J/mol×K	1087.72	Joback Method
cpg	715.43	J/mol×K	1130.05	Joback Method
cpg	719.44	J/mol×K	1172.39	Joback Method
cpg	722.52	J/mol×K	1214.73	Joback Method
dvisc	0.0002084	Pa×s	650.69	Joback Method

dvisc	0.0001413	Pa×s	702.36	Joback Method
dvisc	0.0001011	Pa×s	754.03	Joback Method
dvisc	0.0000755	Pa×s	805.70	Joback Method
dvisc	0.0000584	Pa×s	857.37	Joback Method
dvisc	0.0000465	Pa×s	909.04	Joback Method
dvisc	0.0000379	Pa×s	960.71	Joback Method

Sources

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=U363628&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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