

Dimethylmalonic acid, di(2,5-dichlorophenyl) ester

Inchi:	InChI=1S/C17H12Cl4O4/c1-17(2,15(22)24-13-7-9(18)3-5-11(13)20)16(23)25-14-8-10(19)
InchiKey:	VBEFTBIJHKPMM-UHFFFAOYSA-N
Formula:	C17H12Cl4O4
SMILES:	CC(C)(C(=O)Oc1cc(Cl)ccc1Cl)C(=O)Oc1cc(Cl)ccc1Cl
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	2678.00		NIST Webbook
rinpol	2678.00		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/molxK	960.71	Joback Method
cpg	697.31	J/molxK	1003.05	Joback Method
cpg	704.42	J/molxK	1045.38	Joback Method
cpg	710.44	J/molxK	1087.72	Joback Method
cpg	715.43	J/molxK	1130.05	Joback Method
cpg	719.44	J/molxK	1172.39	Joback Method
cpg	722.52	J/molxK	1214.73	Joback Method
dvisc	0.0002084	Paxs	650.69	Joback Method

dvisc	0.0001413	Paxs	702.36	Joback Method
dvisc	0.0001011	Paxs	754.03	Joback Method
dvisc	0.0000755	Paxs	805.70	Joback Method
dvisc	0.0000584	Paxs	857.37	Joback Method
dvisc	0.0000465	Paxs	909.04	Joback Method
dvisc	0.0000379	Paxs	960.71	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U363696&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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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