Dimethylmalonic acid, di(2,4,5-trichlorophenyl) ester

Inchi: InChI=1S/C17H10Cl6O4/c1-17(2,15(24)26-13-5-9(20)7(18)3-11(13)22)16(25)27-14-6-10
InchiKey: PCDWNRJWLKVPGO-UHFFFAOYSA-N
Formula: C17H10Cl6O4
SMILES: CC(C)(C(=O)Oc1cc(Cl)c(Cl)cc1Cl)C(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 490.98

Physical Properties

Property code	Value	Unit	Source
gf	-277.28	kJ/mol	Joback Method
hf	-582.76	kJ/mol	Joback Method
hfus	48.88	kJ/mol	Joback Method
hvap	105.29	kJ/mol	Joback Method
log10ws	-8.04		Crippen Method
logp	7.144		Crippen Method
mcvol	291.190	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	3088.00		NIST Webbook
rinpol	3088.00		NIST Webbook
tb	1045.53	K	Joback Method
tc	1306.14	K	Joback Method
tf	735.57	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.25	J/mol×K	1045.53	Joback Method
cpg	719.76	J/mol×K	1088.96	Joback Method
cpg	724.14	J/mol×K	1132.40	Joback Method
cpg	727.44	J/mol×K	1175.83	Joback Method
cpg	729.70	J/mol×K	1219.27	Joback Method
cpg	730.97	J/mol×K	1262.70	Joback Method
cpg	731.29	J/mol×K	1306.14	Joback Method
dvisc	0.0001224	Pa×s	735.57	Joback Method

dvisc	0.0000882	Pa×s	787.23	Joback Method
dvisc	0.0000662	Pa×s	838.89	Joback Method
dvisc	0.0000513	Pa×s	890.55	Joback Method
dvisc	0.0000409	Pa×s	942.21	Joback Method
dvisc	0.0000334	Pa×s	993.87	Joback Method
dvisc	0.0000278	Pa×s	1045.53	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=U363855&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