Dimethylmalonic acid, 2,3-dichlorophenyl hexyl ester

Inchi: InChI=1S/C17H22Cl2O4/c1-4-5-6-7-11-22-15(20)17(2,3)16(21)23-13-10-8-9-12(18)14(13

InchiKey: CAEKXFNNLFPQMO-UHFFFAOYSA-N

Formula: C17H22Cl2O4

SMILES: CCCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 361.26

Physical Properties

Property code	Value	Unit	Source
gf	-303.45	kJ/mol	Joback Method
hf	-710.45	kJ/mol	Joback Method
hfus	39.60	kJ/mol	Joback Method
hvap	82.82	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.048		Crippen Method
mcvol	265.990	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	2262.00		NIST Webbook
tb	849.21	K	Joback Method
tc	1065.57	K	Joback Method
tf	539.39	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.53	J/mol×K	849.21	Joback Method
cpg	769.72	J/mol×K	885.27	Joback Method
cpg	781.86	J/mol×K	921.33	Joback Method
cpg	792.96	J/mol×K	957.39	Joback Method
cpg	803.08	J/mol×K	993.45	Joback Method
cpg	812.24	J/mol×K	1029.51	Joback Method
cpg	820.49	J/mol×K	1065.57	Joback Method
dvisc	0.0004241	Pa×s	539.39	Joback Method
dvisc	0.0002541	Pa×s	591.03	Joback Method

dvisc	0.0001653	Pa×s	642.66	Joback Method
dvisc	0.0001147	Pa×s	694.30	Joback Method
dvisc	0.0000837	Pa×s	745.94	Joback Method
dvisc	0.0000636	Pa×s	797.57	Joback Method
dvisc	0.0000500	Pa×s	849.21	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=U363624&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