Diethylmalonic acid, monochloride, 2,3-dichlorophenyl ester

Inchi: InChI=1S/C13H13Cl3O3/c1-3-13(4-2,11(16)17)12(18)19-9-7-5-6-8(14)10(9)15/h5-7H,3-4

InchiKey: QHRQKQSKJXHOJW-UHFFFAOYSA-N

Formula: C13H13Cl3O3

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 323.60

Physical Properties

Property code	Value	Unit	Source
gf	-244.06	kJ/mol	Joback Method
hf	-511.41	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	75.89	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.471		Crippen Method
mcvol	216.000	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
tb	772.70	K	Joback Method
tc	1004.44	K	Joback Method
tf	502.00	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.26	J/mol×K	772.70	Joback Method
cpg	546.37	J/mol×K	811.32	Joback Method
cpg	556.55	J/mol×K	849.95	Joback Method
cpg	565.85	J/mol×K	888.57	Joback Method
cpg	574.33	J/mol×K	927.20	Joback Method
cpg	582.02	J/mol×K	965.82	Joback Method
cpg	588.99	J/mol×K	1004.44	Joback Method
dvisc	0.0007441	Pa×s	502.00	Joback Method

dvisc	0.0004671	Pa×s	547.12	Joback Method
dvisc	0.0003148	Pa×s	592.23	Joback Method
dvisc	0.0002243	Pa×s	637.35	Joback Method
dvisc	0.0001672	Pa×s	682.47	Joback Method
dvisc	0.0001292	Pa×s	727.58	Joback Method
dvisc	0.0001029	Pa×s	772.70	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=U370046&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