Diethylmalonic acid, monochloride, 2-chlorophenyl ester

Inchi: InChI=1S/C13H14Cl2O3/c1-3-13(4-2,11(15)16)12(17)18-10-8-6-5-7-9(10)14/h5-8H,3-4H

InchiKey: NNXBFWGWMZXTHU-UHFFFAOYSA-N

Formula: C13H14Cl2O3

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1ccccc1Cl

Mol. weight [g/mol]: 289.15

Physical Properties

Property code	Value	Unit	Source
gf	-222.50	kJ/mol	Joback Method
hf	-484.20	kJ/mol	Joback Method
hfus	28.44	kJ/mol	Joback Method
hvap	70.85	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.817		Crippen Method
mcvol	203.760	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	730.29	K	Joback Method
tc	958.68	K	Joback Method
tf	459.56	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.54	J/mol×K	730.29	Joback Method
cpg	567.14	J/mol×K	920.61	Joback Method
cpg	558.38	J/mol×K	882.55	Joback Method
cpg	548.79	J/mol×K	844.48	Joback Method
cpg	538.33	J/mol×K	806.42	Joback Method
cpg	526.93	J/mol×K	768.35	Joback Method
cpg	575.13	J/mol×K	958.68	Joback Method
dvisc	0.0001180	Pa×s	730.29	Joback Method

dvisc	0.0001507	Pa×s	685.17	Joback Method
dvisc	0.0001992	Pa×s	640.05	Joback Method
dvisc	0.0002748	Pa×s	594.92	Joback Method
dvisc	0.0003996	Pa×s	549.80	Joback Method
dvisc	0.0006213	Pa×s	504.68	Joback Method
dvisc	0.0010535	Pa×s	459.56	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=U369630&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