Diethylmalonic acid, di(2-chlorophenyl) ester

Inchi: InChI=1S/C19H18Cl2O4/c1-3-19(4-2,17(22)24-15-11-7-5-9-13(15)20)18(23)25-16-12-8-6
InchiKey: IIFRVQWQQKNIHR-UHFFFAOYSA-N
Formula: C19H18Cl2O4
SMILES: CCC(CC)(C(=O)Oc1ccccc1Cl)C(=O)Oc1ccccc1Cl
Mol. weight [g/mol]: 381.25

Physical Properties

Property code	Value	Unit	Source
gf	-174.20	kJ/mol	Joback Method
hf	-515.20	kJ/mol	Joback Method
hfus	38.82	kJ/mol	Joback Method
hvap	89.55	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.311		Crippen Method
mcvol	270.410	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	2589.00		NIST Webbook
tb	921.65	K	Joback Method
tc	1163.19	K	Joback Method
tf	588.35	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.29	J/mol×K	921.65	Joback Method
cpg	779.75	J/mol×K	961.91	Joback Method
cpg	789.99	J/mol×K	1002.16	Joback Method
cpg	799.08	J/mol×K	1042.42	Joback Method
cpg	807.09	J/mol×K	1082.68	Joback Method
cpg	814.09	J/mol×K	1122.94	Joback Method
cpg	820.14	J/mol×K	1163.19	Joback Method
dvisc	0.0003021	Pa×s	588.35	Joback Method
dvisc	0.0001840	Pa×s	643.90	Joback Method

dvisc	0.0001212	Pa×s	699.45	Joback Method
dvisc	0.0000849	Pa×s	755.00	Joback Method
dvisc	0.0000624	Pa×s	810.55	Joback Method
dvisc	0.0000478	Pa×s	866.10	Joback Method
dvisc	0.0000378	Pa×s	921.65	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=U369629&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