Dimethylmalonic acid, di(2-chloro-6-fluorophenyl) ester

Inchi: InChI=1S/C17H12Cl2F2O4/c1-17(2,15(22)24-13-9(18)5-3-7-11(13)20)16(23)25-14-10(19

InchiKey: SPBYYSCSYSLWKH-UHFFFAOYSA-N

Formula: C17H12Cl2F2O4

SMILES: CC(C)(C(=O)Oc1c(F)cccc1Cl)C(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 389.18

Physical Properties

Property code	Value	Unit	Source
gf	-599.92	kJ/mol	Joback Method
hf	-889.08	kJ/mol	Joback Method
hfus	39.03	kJ/mol	Joback Method
hvap	84.79	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.809		Crippen Method
mcvol	245.770	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	2462.00		NIST Webbook
rinpol	2462.00		NIST Webbook
tb	884.39	K	Joback Method
tc	1117.68	K	Joback Method
tf	592.03	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.87	J/mol×K	884.39	Joback Method
cpg	677.84	J/mol×K	923.27	Joback Method
cpg	686.72	J/mol×K	962.15	Joback Method
cpg	694.55	J/mol×K	1001.04	Joback Method
cpg	701.37	J/mol×K	1039.92	Joback Method
cpg	707.22	J/mol×K	1078.80	Joback Method
cpg	712.15	J/mol×K	1117.68	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=U361969&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
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