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

Inchi: InChI=1S/C19H16Cl2F2O4/c1-3-19(4-2,17(24)26-15-11(20)7-5-9-13(15)22)18(25)27-16-

InchiKey: NMTHDQXANNUKEL-UHFFFAOYSA-N

Formula: C19H16Cl2F2O4

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

Mol. weight [g/mol]: 417.23

Physical Properties

Property code	Value	Unit	Source
gf	-583.08	kJ/mol	Joback Method
hf	-930.36	kJ/mol	Joback Method
hfus	44.21	kJ/mol	Joback Method
hvap	89.24	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.589		Crippen Method
mcvol	273.950	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	2563.00		NIST Webbook
rinpol	2563.00		NIST Webbook
tb	930.15	K	Joback Method
tc	1159.90	K	Joback Method
tf	614.57	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.42	J/mol×K	930.15	Joback Method
cpg	789.81	J/mol×K	968.44	Joback Method
cpg	799.08	J/mol×K	1006.73	Joback Method
cpg	807.27	J/mol×K	1045.03	Joback Method
cpg	814.43	J/mol×K	1083.32	Joback Method
cpg	820.60	J/mol×K	1121.61	Joback Method
cpg	825.83	J/mol×K	1159.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U369687&Units=SI

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