Diethylmalonic acid, di(2-fluorophenyl) ester

Inchi: InChI=1S/C19H18F2O4/c1-3-19(4-2,17(22)24-15-11-7-5-9-13(15)20)18(23)25-16-12-8-6
InchiKey: KXXOGJAJLUYOJM-UHFFFAOYSA-N
Formula: C19H18F2O4
SMILES: CCC(CC)(C(=O)Oc1ccccc1F)C(=O)Oc1ccccc1F
Mol. weight [g/mol]: 348.34

Physical Properties

Property code	Value	Unit	Source
gf	-539.96	kJ/mol	Joback Method
hf	-875.94	kJ/mol	Joback Method
hfus	36.59	kJ/mol	Joback Method
hvap	79.15	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.282		Crippen Method
mcvol	249.470	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	2203.00		NIST Webbook
tb	845.33	K	Joback Method
tc	1066.37	K	Joback Method
tf	529.69	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.42	J/mol×K	845.33	Joback Method
cpg	752.57	J/mol×K	882.17	Joback Method
cpg	764.56	J/mol×K	919.01	Joback Method
cpg	775.43	J/mol×K	955.85	Joback Method
cpg	785.25	J/mol×K	992.69	Joback Method
cpg	794.05	J/mol×K	1029.53	Joback Method
cpg	801.89	J/mol×K	1066.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370143&Units=SI
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

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