Diethylmalonic acid, monochloride, 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C13H12ClF3O3/c1-3-13(4-2,11(14)18)12(19)20-8-6-5-7(15)9(16)10(8)17/h5-6H

InchiKey: LIZWWFUSPVUKPS-UHFFFAOYSA-N

Formula: C13H12ClF3O3

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 308.68

Physical Properties

Property code	Value	Unit	Source
gf	-814.26	kJ/mol	Joback Method
hf	-1079.73	kJ/mol	Joback Method
hfus	32.71	kJ/mol	Joback Method
hvap	65.33	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.581		Crippen Method
mcvol	196.830	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1579.00		NIST Webbook
tb	700.63	K	Joback Method
tc	901.75	K	Joback Method
tf	456.45	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.05	J/mol×K	700.63	Joback Method
cpg	523.58	J/mol×K	734.15	Joback Method
cpg	534.34	J/mol×K	767.67	Joback Method
cpg	544.35	J/mol×K	801.19	Joback Method
cpg	553.64	J/mol×K	834.71	Joback Method
cpg	562.24	J/mol×K	868.23	Joback Method
cpg	570.18	J/mol×K	901.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370705&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