Diethylmalonic acid, monochloride, 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C14H13ClF4O3/c1-3-13(4-2,11(15)20)12(21)22-9-7-5-6-8(10(9)16)14(17,18)19

InchiKey: CZMOIYYCTPLDED-UHFFFAOYSA-N

Formula: C14H13ClF4O3

SMILES: CCC(CC)(C(=O)Cl)C(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 340.70

Physical Properties

Property code	Value	Unit	Source
gf	-988.18	kJ/mol	Joback Method
hf	-1293.76	kJ/mol	Joback Method
hfus	31.35	kJ/mol	Joback Method
hvap	64.78	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.322		Crippen Method
mcvol	212.690	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	1599.00		NIST Webbook
rinpol	1599.00		NIST Webbook
tb	714.57	K	Joback Method
tc	914.36	K	Joback Method
tf	458.21	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.67	J/mol×K	714.57	Joback Method
cpg	587.56	J/mol×K	747.87	Joback Method
cpg	598.58	J/mol×K	781.17	Joback Method
cpg	608.78	J/mol×K	814.46	Joback Method
cpg	618.22	J/mol×K	847.76	Joback Method
cpg	626.93	J/mol×K	881.06	Joback Method
cpg	634.99	J/mol×K	914.36	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=U370726&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