2,4-Difluorobenzoic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C13H5Cl3F2O2/c14-8-4-10(16)12(5-9(8)15)20-13(19)7-2-1-6(17)3-11(7)18/h1-

InchiKey: JLFBQPLLXJNARA-UHFFFAOYSA-N

Formula: C13H5Cl3F2O2

SMILES: O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1ccc(F)cc1F

Mol. weight [g/mol]: 337.53

Physical Properties

Property code	Value	Unit	Source
gf	-424.08	kJ/mol	Joback Method
hf	-580.18	kJ/mol	Joback Method
hfus	37.10	kJ/mol	Joback Method
hvap	73.07	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.144		Crippen Method
mcvol	194.210	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	2122.00		NIST Webbook
rinpol	2122.00		NIST Webbook
tb	762.22	K	Joback Method
tc	999.55	K	Joback Method
tf	514.81	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.53	J/mol×K	762.22	Joback Method
cpg	450.68	J/mol×K	801.77	Joback Method
cpg	458.99	J/mol×K	841.33	Joback Method
cpg	466.48	J/mol×K	880.88	Joback Method
cpg	473.16	J/mol×K	920.44	Joback Method
cpg	479.06	J/mol×K	959.99	Joback Method
cpg	484.18	J/mol×K	999.55	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=U360563&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