2,5-Difluorobenzoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C13H6Cl2F2O2/c14-10-3-2-8(6-11(10)15)19-13(18)9-5-7(16)1-4-12(9)17/h1-6H

InchiKey: LQGUUHGHXIRVMM-UHFFFAOYSA-N

Formula: C13H6Cl2F2O2

SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)c1cc(F)ccc1F

Mol. weight [g/mol]: 303.09

Physical Properties

Property code	Value	Unit	Source
gf	-402.52	kJ/mol	Joback Method
hf	-552.97	kJ/mol	Joback Method
hfus	33.29	kJ/mol	Joback Method
hvap	68.02	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.491		Crippen Method
mcvol	181.970	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	2043.00		NIST Webbook
rinpol	2043.00		NIST Webbook
tb	719.81	K	Joback Method
tc	953.95	K	Joback Method
tf	472.37	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.27	J/mol×K	719.81	Joback Method
cpg	433.60	J/mol×K	758.83	Joback Method
cpg	443.05	J/mol×K	797.86	Joback Method
cpg	451.67	J/mol×K	836.88	Joback Method
cpg	459.45	J/mol×K	875.90	Joback Method
cpg	466.44	J/mol×K	914.93	Joback Method
cpg	472.65	J/mol×K	953.95	Joback Method

Sources

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=U357585&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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