2,4-Difluorobenzoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C13H3F7O2/c14-4-1-2-5(6(15)3-4)13(21)22-12-10(19)8(17)7(16)9(18)11(12)20

InchiKey: ZDBKOPSCVKQWAX-UHFFFAOYSA-N

Formula: C13H3F7O2

SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)c1ccc(F)cc1F

Mol. weight [g/mol]: 324.15

Physical Properties

Property code	Value	Unit	Source
gf	-1381.60	kJ/mol	Joback Method
hf	-1536.45	kJ/mol	Joback Method
hfus	39.13	kJ/mol	Joback Method
hvap	57.16	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	3.880		Crippen Method
mcvol	166.340	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1454.00		NIST Webbook
rinpol	1454.00		NIST Webbook
tb	656.24	K	Joback Method
tc	843.37	K	Joback Method
tf	453.04	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.36	J/mol×K	656.24	Joback Method
cpg	424.66	J/mol×K	687.43	Joback Method
cpg	433.44	J/mol×K	718.62	Joback Method
cpg	441.69	J/mol×K	749.81	Joback Method
cpg	449.41	J/mol×K	780.99	Joback Method
cpg	456.61	J/mol×K	812.18	Joback Method
cpg	463.27	J/mol×K	843.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360555&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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