2,4-Difluorobenzoic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C13H4Cl4F2O2/c14-7-4-8(15)12(11(17)10(7)16)21-13(20)6-2-1-5(18)3-9(6)19/

InchiKey: JEJOXPHAGVGUNT-UHFFFAOYSA-N

Formula: C13H4Cl4F2O2

SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1ccc(F)cc1F

Mol. weight [g/mol]: 371.98

Physical Properties

Property code	Value	Unit	Source
gf	-445.64	kJ/mol	Joback Method
hf	-607.39	kJ/mol	Joback Method
hfus	40.91	kJ/mol	Joback Method
hvap	78.12	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	5.798		Crippen Method
mcvol	206.450	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	2247.00		NIST Webbook
tb	804.63	K	Joback Method
tc	1044.95	K	Joback Method
tf	557.25	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.01	J/mol×K	804.63	Joback Method
cpg	466.03	J/mol×K	844.68	Joback Method
cpg	473.23	J/mol×K	884.74	Joback Method
cpg	479.62	J/mol×K	924.79	Joback Method
cpg	485.20	J/mol×K	964.84	Joback Method
cpg	490.00	J/mol×K	1004.89	Joback Method
cpg	494.03	J/mol×K	1044.95	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=U360564&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