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

Inchi: InChI=1S/C13HCl4F5O2/c14-2-1-3(15)12(6(17)5(2)16)24-13(23)4-7(18)9(20)11(22)10(21

InchiKey: CDGADYJJBKICNY-UHFFFAOYSA-N

Formula: C13HCl4F5O2

SMILES: O=C(Oc1c(Cl)cc(Cl)c(Cl)c1Cl)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 425.95

Physical Properties

Property code	Value	Unit	Source
gf	-1058.96	kJ/mol	Joback Method
hf	-1230.13	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	77.65	kJ/mol	Joback Method
log10ws	-7.96		Crippen Method
logp	6.215		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	2110.00		NIST Webbook
tb	817.38	K	Joback Method
tc	1035.08	K	Joback Method
tf	596.58	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.73	J/mol×K	817.38	Joback Method
cpg	481.41	J/mol×K	853.66	Joback Method
cpg	487.43	J/mol×K	889.95	Joback Method
cpg	492.78	J/mol×K	926.23	Joback Method
cpg	497.45	J/mol×K	962.51	Joback Method
cpg	501.43	J/mol×K	998.79	Joback Method
cpg	504.71	J/mol×K	1035.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360632&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