Pentafluorobenzoic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C13H2Cl3F5O2/c14-3-1-5(16)6(2-4(3)15)23-13(22)7-8(17)10(19)12(21)11(20)9

InchiKey: MFYDGNNHFUZELW-UHFFFAOYSA-N

Formula: C13H2Cl3F5O2

SMILES: O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 391.50

Physical Properties

Property code	Value	Unit	Source
gf	-1037.40	kJ/mol	Joback Method
hf	-1202.92	kJ/mol	Joback Method
hfus	45.17	kJ/mol	Joback Method
hvap	72.61	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	5.562		Crippen Method
mcvol	199.520	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	1963.00		NIST Webbook
tb	774.97	K	Joback Method
tc	988.56	K	Joback Method
tf	554.14	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.13	J/mol×K	774.97	Joback Method
cpg	466.76	J/mol×K	810.57	Joback Method
cpg	473.73	J/mol×K	846.17	Joback Method
cpg	480.05	J/mol×K	881.77	Joback Method
cpg	485.72	J/mol×K	917.36	Joback Method
cpg	490.72	J/mol×K	952.96	Joback Method
cpg	495.07	J/mol×K	988.56	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=U360631&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