Pentafluorobenzoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C13F10O2/c14-2-1(3(15)5(17)6(18)4(2)16)13(24)25-12-10(22)8(20)7(19)9(21)

InchiKey: ZTQHONLMYPIEDI-UHFFFAOYSA-N

Formula: C13F10O2

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

Mol. weight [g/mol]: 378.12

Physical Properties

Property code	Value	Unit	Source
gf	-1994.92	kJ/mol	Joback Method
hf	-2159.19	kJ/mol	Joback Method
hfus	47.20	kJ/mol	Joback Method
hvap	56.69	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	4.297		Crippen Method
mcvol	171.650	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1342.00		NIST Webbook
tb	668.99	K	Joback Method
tc	840.70	K	Joback Method
tf	492.37	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.32	J/mol×K	668.99	Joback Method
cpg	443.20	J/mol×K	697.61	Joback Method
cpg	450.70	J/mol×K	726.23	Joback Method
cpg	457.79	J/mol×K	754.85	Joback Method
cpg	464.47	J/mol×K	783.46	Joback Method
cpg	470.73	J/mol×K	812.08	Joback Method
cpg	476.56	J/mol×K	840.70	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=U360623&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