Phthalic acid, di(pentafluorophenyl) ester

Inchi: InChI=1S/C20H4F10O4/c21-7-9(23)13(27)17(14(28)10(7)24)33-19(31)5-3-1-2-4-6(5)20(3
InchiKey: XNHCTIRBMWXOHR-UHFFFAOYSA-N
Formula: C20H4F10O4
SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)c1ccccc1C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 498.23

Physical Properties

Property code	Value	Unit	Source
gf	-2067.12	kJ/mol	Joback Method
hf	-2323.41	kJ/mol	Joback Method
hfus	61.77	kJ/mol	Joback Method
hvap	84.37	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	5.516		Crippen Method
mcvol	253.960	ml/mol	McGowan Method
pc	1404.84	kPa	Joback Method
rinpol	2179.00		NIST Webbook
rinpol	2179.00		NIST Webbook
tb	937.10	K	Joback Method
tc	1148.45	K	Joback Method
tf	682.36	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.31	J/mol×K	937.10	Joback Method
cpg	742.78	J/mol×K	972.32	Joback Method
cpg	749.14	J/mol×K	1007.55	Joback Method
cpg	754.37	J/mol×K	1042.77	Joback Method
cpg	758.47	J/mol×K	1078.00	Joback Method
cpg	761.43	J/mol×K	1113.22	Joback Method
cpg	763.23	J/mol×K	1148.45	Joback Method

Sources

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=U356374&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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