Phthalic acid, hexyl pentafluorophenyl ester

Inchi: InChI=1S/C20H17F5O4/c1-2-3-4-7-10-28-19(26)11-8-5-6-9-12(11)20(27)29-18-16(24)14
InchiKey: VSBQWJFDADDQTI-UHFFFAOYSA-N
Formula: C20H17F5O4
SMILES: CCCCCCOC(=O)c1ccccc1C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 416.34

Physical Properties

Property code	Value	Unit	Source
gf	-1157.33	kJ/mol	Joback Method
hf	-1522.04	kJ/mol	Joback Method
hfus	54.28	kJ/mol	Joback Method
hvap	82.86	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	5.338		Crippen Method
mcvol	268.870	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2283.00		NIST Webbook
rinpol	2283.00		NIST Webbook
tb	889.17	K	Joback Method
tc	1093.67	K	Joback Method
tf	590.39	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.97	J/mol×K	889.17	Joback Method
cpg	823.73	J/mol×K	923.25	Joback Method
cpg	834.40	J/mol×K	957.34	Joback Method
cpg	844.00	J/mol×K	991.42	Joback Method
cpg	852.52	J/mol×K	1025.51	Joback Method
cpg	859.98	J/mol×K	1059.59	Joback Method
cpg	866.38	J/mol×K	1093.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356295&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