Pentafluorobenzoic acid, 4-biphenyl ester

Inchi: InChI=1S/C19H9F5O2/c20-14-13(15(21)17(23)18(24)16(14)22)19(25)26-12-8-6-11(7-9-1
InchiKey: ZZIFUUFUMSUZNP-UHFFFAOYSA-N
Formula: C19H9F5O2
SMILES: O=C(Oc1ccc(-c2ccccc2)cc1)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 364.27

Physical Properties

Property code	Value	Unit	Source
gf	-819.42	kJ/mol	Joback Method
hf	-1020.07	kJ/mol	Joback Method
hfus	42.94	kJ/mol	Joback Method
hvap	73.76	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	5.268		Crippen Method
mcvol	223.580	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	2271.00		NIST Webbook
tb	816.68	K	Joback Method
tc	1036.39	K	Joback Method
tf	533.38	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.05	J/mol×K	816.68	Joback Method
cpg	632.54	J/mol×K	853.30	Joback Method
cpg	643.00	J/mol×K	889.92	Joback Method
cpg	652.47	J/mol×K	926.53	Joback Method
cpg	660.98	J/mol×K	963.15	Joback Method
cpg	668.56	J/mol×K	999.77	Joback Method
cpg	675.25	J/mol×K	1036.39	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=U360633&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