3-Fluorobenzoic acid, 4-biphenyl ester

Inchi: InChI=1S/C19H13FO2/c20-17-8-4-7-16(13-17)19(21)22-18-11-9-15(10-12-18)14-5-2-1-3
InchiKey: NEJFXILJSJCKGI-UHFFFAOYSA-N
Formula: C19H13FO2
SMILES: O=C(Oc1ccc(-c2ccccc2)cc1)c1cccc(F)c1
Mol. weight [g/mol]: 292.30

Physical Properties

Property code	Value	Unit	Source
gf	-1.66	kJ/mol	Joback Method
hf	-189.75	kJ/mol	Joback Method
hfus	32.18	kJ/mol	Joback Method
hvap	74.38	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	4.712		Crippen Method
mcvol	216.500	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	2530.00		NIST Webbook
tb	799.68	K	Joback Method
tc	1052.32	K	Joback Method
tf	480.94	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.32	J/mol×K	799.68	Joback Method
cpg	610.61	J/mol×K	841.79	Joback Method
cpg	623.49	J/mol×K	883.89	Joback Method
cpg	635.07	J/mol×K	926.00	Joback Method
cpg	645.42	J/mol×K	968.10	Joback Method
cpg	654.62	J/mol×K	1010.21	Joback Method
cpg	662.76	J/mol×K	1052.32	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=U355669&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