3-Chloro-2-fluorobenzoic acid, 2-biphenyl ester

Inchi: InChI=1S/C19H12ClFO2/c20-16-11-6-10-15(18(16)21)19(22)23-17-12-5-4-9-14(17)13-7-

InchiKey: SQBCNBGRVHHVRK-UHFFFAOYSA-N

Formula: C19H12ClFO2

SMILES: O=C(Oc1ccccc1-c1ccccc1)c1cccc(Cl)c1F

Mol. weight [g/mol]: 326.75

Physical Properties

Property code	Value	Unit	Source
gf	-23.22	kJ/mol	Joback Method
hf	-216.96	kJ/mol	Joback Method
hfus	35.99	kJ/mol	Joback Method
hvap	79.43	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	5.365		Crippen Method
mcvol	228.740	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
rinpol	2446.00		NIST Webbook
rinpol	2446.00		NIST Webbook
tb	842.09	K	Joback Method
tc	1097.09	K	Joback Method
tf	523.38	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.09	J/mol×K	842.09	Joback Method
cpg	629.76	J/mol×K	884.59	Joback Method
cpg	641.10	J/mol×K	927.09	Joback Method
cpg	651.21	J/mol×K	969.59	Joback Method
cpg	660.15	J/mol×K	1012.09	Joback Method
cpg	668.00	J/mol×K	1054.59	Joback Method
cpg	674.85	J/mol×K	1097.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357335&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

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