BENZOIC ACID, 2-FLUORO-, 4-BIPHENYLYL ESTER

Other names: 2-Fluorobenzoic acid, 4-biphenyl ester
Inchi: InChI=1S/C19H13FO2/c20-18-9-5-4-8-17(18)19(21)22-16-12-10-15(11-13-16)14-6-2-1-3
InchiKey: MJUWGKGNELOGFC-UHFFFAOYSA-N
Formula: C19H13FO2
SMILES: O=C(Oc1ccc(-c2ccccc2)cc1)c1ccccc1F
Mol. weight [g/mol]: 292.31

Physical Properties

Property code	Value	Unit	Source
hf	-259.28	kJ/mol	Cheméo Relay (1.0)
hfus	32.18	kJ/mol	Joback Method
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-5.94		Cheméo Relay (1.0)
logp	4.712		Crippen Method
mcvol	216.500	ml/mol	McGowan Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook
tb	664.14	K	Cheméo Relay (1.0)
tf	379.51	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C300405861&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point