

2,4-Difluorobenzoic acid, 4-biphenyl ester

Inchi:	InChI=1S/C19H12F2O2/c20-15-8-11-17(18(21)12-15)19(22)23-16-9-6-14(7-10-16)13-4-2
InchiKey:	YMIADCHHVQVMNO-UHFFFAOYSA-N
Formula:	C19H12F2O2
SMILES:	O=C(Oc1ccc(-c2ccccc2)cc1)c1ccc(F)cc1F
Mol. weight [g/mol]:	310.29

Physical Properties

Property code	Value	Unit	Source
gf	-206.10	kJ/mol	Joback Method
hf	-397.33	kJ/mol	Joback Method
hfus	34.87	kJ/mol	Joback Method
hvap	74.22	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	4.851		Crippen Method
mvol	218.270	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	2465.00		NIST Webbook
tb	803.93	K	Joback Method
tc	1047.01	K	Joback Method
tf	494.05	K	Joback Method
vc	0.836	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.57	J/mol×K	803.93	Joback Method
cpg	616.06	J/mol×K	844.44	Joback Method
cpg	628.26	J/mol×K	884.96	Joback Method
cpg	639.25	J/mol×K	925.47	Joback Method
cpg	649.10	J/mol×K	965.98	Joback Method
cpg	657.85	J/mol×K	1006.50	Joback Method
cpg	665.60	J/mol×K	1047.01	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=U360565&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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

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