

1,1'-Biphenyl, 4,4'-difluoro-

Other names:	4,4'-Difluorobiphenyl Biphenyl, 4,4'-difluoro- 4,4'-Difluorodiphenyl
Inchi:	InChI=1S/C12H8F2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8H
InchiKey:	PZDAAZQDQJGXSW-UHFFFAOYSA-N
Formula:	C12H8F2
SMILES:	Fc1ccc(-c2ccc(F)cc2)cc1
Mol. weight [g/mol]:	190.19
CAS:	398-23-2

Physical Properties

Property code	Value	Unit	Source
chs	-5927.10 ± 0.92	kJ/mol	NIST Webbook
gf	-133.90	kJ/mol	Joback Method
hf	-205.40 ± 4.70	kJ/mol	NIST Webbook
hfs	-296.60 ± 2.20	kJ/mol	NIST Webbook
hfus	20.30	kJ/mol	Joback Method
hsub	91.20 ± 4.20	kJ/mol	NIST Webbook
hvap	46.55	kJ/mol	Joback Method
ie	8.00 ± 0.02	eV	NIST Webbook
log10ws	-4.74		Crippen Method
logp	3.632		Crippen Method
mcvol	135.960	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	234.08		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	233.78		NIST Webbook
ripol	233.87		NIST Webbook
ripol	233.87		NIST Webbook
ss	237.59	J/molxK	NIST Webbook
tb	527.70	K	NIST Webbook
tc	762.30	K	Joback Method
tf	363.10 ± 2.00	K	NIST Webbook
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.88	J/mol×K	535.82	Joback Method
cpg	308.80	J/mol×K	573.57	Joback Method
cpg	321.75	J/mol×K	611.31	Joback Method
cpg	333.77	J/mol×K	649.06	Joback Method
cpg	344.91	J/mol×K	686.81	Joback Method
cpg	355.21	J/mol×K	724.55	Joback Method
cpg	364.72	J/mol×K	762.30	Joback Method
cps	222.77	J/mol×K	298.15	NIST Webbook
hvapt	91.20	kJ/mol	298.15	NIST Webbook
svapt	305.00	J/mol×K	298.15	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C398232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature

ie:	Ionization energy
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
ripol:	Polar retention indices
ss:	Solid phase molar entropy at standard conditions
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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