2,2'-Difluorobiphenyl

Other names:	1,1'-Biphenyl, 2,2'-difluoro- 2,2'-Difluorodiphenyl Biphenyl, 2,2'-difluoro 2,2'-difluoro-1,1'-biphenyl
Inchi:	InChI=1S/C12H8F2/c13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)14/h1-8H
InchiKey:	PXFIPIAXFGAEMJ-UHFFFAOYSA-N
Formula:	C12H8F2
SMILES:	Fc1ccccc1-c1ccccc1F
Mol. weight [g/mol]:	190.19
CAS:	388-82-9

Physical Properties

Property code	Value	Unit	Source
chs	-5927.85 ± 0.63	kJ/mol	NIST Webbook
gf	-133.90	kJ/mol	Joback Method
hf	-200.70 ± 4.70	kJ/mol	NIST Webbook
hfs	-295.80 ± 2.10	kJ/mol	NIST Webbook
hfus	20.30	kJ/mol	Joback Method
hsub	95.00 ± 4.20	kJ/mol	NIST Webbook
hsub	95.00 ± 4.20	kJ/mol	NIST Webbook
hvap	46.55	kJ/mol	Joback Method
ie	8.35 ± 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	229.47		NIST Webbook
rinpol	229.19		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook
ripol	226.78		NIST Webbook
ripol	226.78		NIST Webbook
tb	535.82	K	Joback Method
tc	762.30	K	Joback Method
tf	304.06	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.21	J/mol×K	724.55	Joback Method
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	364.72	J/mol×K	762.30	Joback Method
hsubt	95.10	kJ/mol	310.00	NIST Webbook

Sources

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=C388829&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas 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
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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