

# P,p'-biphenol, 2,2'-difluoro-

<b>Inchi:</b>	InChI=1S/C12H8F2O2/c13-9-5-7(1-3-11(9)15)8-2-4-12(16)10(14)6-8/h1-6,15-16H
<b>InchiKey:</b>	OXGQXNQNP-UHFFFAOYSA-N
<b>Formula:</b>	C12H8F2O2
<b>SMILES:</b>	Oc1ccc(-c2ccc(O)c(F)c2)cc1F
<b>Mol. weight [g/mol]:</b>	222.19
<b>CAS:</b>	396-86-1

## Physical Properties

Property code	Value	Unit	Source
gf	-443.14	kJ/mol	Joback Method
hf	-587.73	kJ/mol	Joback Method
hfus	31.87	kJ/mol	Joback Method
hvap	72.58	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.043		Crippen Method
mvol	147.700	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
tb	697.06	K	Joback Method
tc	942.09	K	Joback Method
tf	527.50	K	Joback Method
vc	0.460	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.51	J/mol×K	697.06	Joback Method
cpg	396.76	J/mol×K	737.90	Joback Method
cpg	406.36	J/mol×K	778.74	Joback Method
cpg	415.47	J/mol×K	819.57	Joback Method
cpg	424.28	J/mol×K	860.41	Joback Method
cpg	432.93	J/mol×K	901.25	Joback Method
cpg	441.60	J/mol×K	942.09	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C396861&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C396861&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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