

1,1'-Biphenyl, 4-fluoro-

Other names:	Biphenyl, 4-fluoro- p-Fluorodiphenyl 4-Fluorobiphenyl p-Fluorobiphenyl
Inchi:	InChI=1S/C12H9F/c13-12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9H
InchiKey:	RUYZJEIKQYLEGZ-UHFFFAOYSA-N
Formula:	C12H9F
SMILES:	Fc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	172.20
CAS:	324-74-3

Physical Properties

Property code	Value	Unit	Source
gf	70.54	kJ/mol	Joback Method
hf	-25.53	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method
hvap	46.70	kJ/mol	Joback Method
ie	8.00 ± 0.02	eV	NIST Webbook
log10ws	-4.41		Crippen Method
logp	3.493		Crippen Method
mcvol	134.190	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	1357.00		NIST Webbook
rinpol	233.89		NIST Webbook
rinpol	1357.00		NIST Webbook
rinpol	233.89		NIST Webbook
rinpol	233.59		NIST Webbook
ripol	230.04		NIST Webbook
ripol	230.04		NIST Webbook
tb	583.00	K	NIST Webbook
tb	583.20	K	NIST Webbook
tc	769.28	K	Joback Method
tf	290.95	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.80	J/mol×K	531.57	Joback Method
cpg	301.89	J/mol×K	571.19	Joback Method
cpg	315.84	J/mol×K	610.81	Joback Method
cpg	328.71	J/mol×K	650.43	Joback Method
cpg	340.58	J/mol×K	690.05	Joback Method
cpg	351.50	J/mol×K	729.66	Joback Method
cpg	361.52	J/mol×K	769.28	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=C324743&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
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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