

[1,1'-Biphenyl]-4-carboxaldehyde

Other names:	4-Biphenylcarboxaldehyde p-Biphenylcarboxaldehyde p-Biphenylaldehyde p-Phenylbenzaldehyde Biphenyl-4-carboxaldehyde 4-Biphenylaldehyde 4-Biphenylcarboxaldehyde 4-Phenylbenzaldehyde 4-Biphenylcarboxaldehyde p-Biphenylaldehyde 4-Formylbiphenyl 4-Formyl-1,1'-biphenyl NSC 46066 Benzaldehyde, p-phenyl-
Inchi:	InChI=1S/C13H10O/c14-10-11-6-8-13(9-7-11)12-4-2-1-3-5-12/h1-10H
InchiKey:	ISDBWOPVZKNQDW-UHFFFAOYSA-N
Formula:	C13H10O
SMILES:	O=Cc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	182.22
CAS:	3218-36-8

Physical Properties

Property code	Value	Unit	Source
gf	174.25	kJ/mol	Joback Method
hf	64.36	kJ/mol	Joback Method
hfus	19.41	kJ/mol	Joback Method
hvap	56.47	kJ/mol	Joback Method
ie	8.47 ± 0.03	eV	NIST Webbook
log10ws	-4.32		Crippen Method
logp	3.166		Crippen Method
mcvol	148.080	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
rinpol	1673.00		NIST Webbook
tb	603.84	K	Joback Method
tc	851.33	K	Joback Method
tf	343.63	K	Joback Method
vc	0.565	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.32	J/molxK	603.84	Joback Method
cpg	356.89	J/molxK	645.09	Joback Method
cpg	370.27	J/molxK	686.34	Joback Method
cpg	382.53	J/molxK	727.59	Joback Method
cpg	393.76	J/molxK	768.84	Joback Method
cpg	404.01	J/molxK	810.08	Joback Method
cpg	413.37	J/molxK	851.33	Joback Method
dvisc	0.0019888	Paxs	343.63	Joback Method
dvisc	0.0011266	Paxs	387.00	Joback Method
dvisc	0.0007156	Paxs	430.37	Joback Method
dvisc	0.0004940	Paxs	473.74	Joback Method
dvisc	0.0003628	Paxs	517.10	Joback Method
dvisc	0.0002795	Paxs	560.47	Joback Method
dvisc	0.0002236	Paxs	603.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	457.20	K	1.50	NIST Webbook

Sources

- NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3218368&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

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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