

4,4'-Biphenylbis(glyoxal-2-hydrate)

Inchi:	InChI=1S/C16H14O6/c17-13(15(19)20)11-5-1-9(2-6-11)10-3-7-12(8-4-10)14(18)16(21)22
InchiKey:	DDPNUFITOMENNU-UHFFFAOYSA-N
Formula:	C16H14O6
SMILES:	O=C(c1ccc(-c2ccc(C(=O)C(O)O)cc2)cc1)C(O)O
Mol. weight [g/mol]:	302.28
CAS:	1094-85-5

Physical Properties

Property code	Value	Unit	Source
gf	-520.60	kJ/mol	Joback Method
hf	-768.09	kJ/mol	Joback Method
hfus	37.00	kJ/mol	Joback Method
hvap	136.52	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	0.340		Crippen Method
mcvol	215.400	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
tb	1104.38	K	Joback Method
tc	1355.51	K	Joback Method
tf	661.10	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.65	J/mol×K	1104.38	Joback Method
cpg	681.04	J/mol×K	1146.23	Joback Method
cpg	686.82	J/mol×K	1188.09	Joback Method
cpg	692.06	J/mol×K	1229.94	Joback Method
cpg	696.87	J/mol×K	1271.80	Joback Method
cpg	701.32	J/mol×K	1313.65	Joback Method
cpg	705.51	J/mol×K	1355.51	Joback Method
dvisc	0.0000058	Pa×s	661.10	Joback Method
dvisc	0.0000014	Pa×s	734.98	Joback Method

dvisc	0.0000005	Pa×s	808.86	Joback Method
dvisc	0.0000002	Pa×s	882.74	Joback Method
dvisc	7.8005254e-08	Pa×s	956.62	Joback Method
dvisc	3.9064391e-08	Pa×s	1030.50	Joback Method
dvisc	2.1459643e-08	Pa×s	1104.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1094855&Units=SI
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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/12-320-2/4-4-Biphenylbis-glyoxal-2-hydrate.pdf>

Generated by Cheméo on 2025-12-05 14:50:09.568714225 +0000 UTC m=+4694407.098754879.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.