

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

Other names:	4-(Hydroxymethyl)biphenyl 4-Biphenylmethanol 4-Phenylbenzyl alcohol 4-biphenylmethanol 4HMB Biphenyl-4-methanol NSC 233860 NSC 84169 p-phenylbenzyl alcohol
Inchi:	InChI=1S/C13H12O/c14-10-11-6-8-13(9-7-11)12-4-2-1-3-5-12/h1-9,14H,10H2
InchiKey:	AXCHZLOJGKSWLV-UHFFFAOYSA-N
Formula:	C13H12O
SMILES:	<chem>OCC1ccc(-c2ccccc2)cc1</chem>
Mol. weight [g/mol]:	184.23
CAS:	3597-91-9

Physical Properties

Property code	Value	Unit	Source
gf	136.95	kJ/mol	Joback Method
hf	-2.29	kJ/mol	Joback Method
hfus	27.00	kJ/mol	Thermochemistry of 2- and 4-biphenylmethanol
hsub	107.30 ± 1.80	kJ/mol	NIST Webbook
hvap	66.42	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	2.846		Crippen Method
mcvol	152.380	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
tb	647.36	K	Joback Method
tc	872.00	K	Joback Method
tf	362.45	K	Joback Method
vc	0.567	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.62	J/molxK	647.36	Joback Method
cpg	390.71	J/molxK	684.80	Joback Method
cpg	402.84	J/molxK	722.24	Joback Method
cpg	414.08	J/molxK	759.68	Joback Method
cpg	424.47	J/molxK	797.12	Joback Method
cpg	434.08	J/molxK	834.56	Joback Method
cpg	442.96	J/molxK	872.00	Joback Method
dvisc	0.0010619	Paxs	409.94	Joback Method
dvisc	0.0030194	Paxs	362.45	Joback Method
dvisc	0.0004640	Paxs	457.42	Joback Method
dvisc	0.0002369	Paxs	504.90	Joback Method
dvisc	0.0001358	Paxs	552.39	Joback Method
dvisc	0.0000850	Paxs	599.88	Joback Method
dvisc	0.0000570	Paxs	647.36	Joback Method
hfust	27.00	kJ/mol	375.50	NIST Webbook
hsubt	105.70 ± 1.80	kJ/mol	349.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of 2- and 4-biphenylmethanol: Joback Method:	https://www.doi.org/10.1016/j.jct.2007.03.002 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=C3597919&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

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