

[1,1'-Biphenyl]-2-ol, 5-(1,1-dimethylethyl)-

Other names:	Phenol, 4-tert-butyl-2-phenyl- 2-Biphenylol, 5-tert-butyl- 2-Phenyl-4-tert-butylphenol 4-tert-Butyl-2-phenylphenol 5-tert-Butyl-2-biphenol 5-Tert-butyl[1,1'-biphenyl]-2-ol 5-(1,1-dimethylethyl)[1,1'-biphenyl]-2-ol
Inchi:	InChI=1S/C16H18O/c1-16(2,3)13-9-10-15(17)14(11-13)12-7-5-4-6-8-12/h4-11,17H,1-3H
InchiKey:	IYPYKRAEQZVXSC-UHFFFAOYSA-N
Formula:	C16H18O
SMILES:	CC(C)(C)c1ccc(O)c(-c2ccccc2)c1
Mol. weight [g/mol]:	226.31
CAS:	577-92-4

Physical Properties

Property code	Value	Unit	Source
gf	147.25	kJ/mol	Joback Method
hf	-98.04	kJ/mol	Joback Method
hfus	23.26	kJ/mol	Joback Method
hvap	68.14	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.357		Crippen Method
mcvol	194.650	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
tb	701.21	K	Joback Method
tc	954.53	K	Joback Method
tf	449.58	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	531.18	J/mol×K	701.21	Joback Method
cpg	547.84	J/mol×K	743.43	Joback Method
cpg	563.23	J/mol×K	785.65	Joback Method
cpg	577.54	J/mol×K	827.87	Joback Method
cpg	590.95	J/mol×K	870.09	Joback Method
cpg	603.66	J/mol×K	912.31	Joback Method
cpg	615.84	J/mol×K	954.53	Joback Method
dvisc	0.0004476	Pa×s	449.58	Joback Method
dvisc	0.0001875	Pa×s	491.52	Joback Method
dvisc	0.0000900	Pa×s	533.46	Joback Method
dvisc	0.0000481	Pa×s	575.39	Joback Method
dvisc	0.0000280	Pa×s	617.33	Joback Method
dvisc	0.0000175	Pa×s	659.27	Joback Method
dvisc	0.0000115	Pa×s	701.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C577924&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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