[1,1'-Biphenyl]-4-ol, 3,5-bis(1,1-dimethylethyl)-

Other names: 2,6-Bis(1,1-dimethylethyl)-4-phenylphenol
2,6-di-tert-butyl-4-phenylphenol
Inchi: InChI=1S/C20H26O/c1-19(2,3)16-12-15(14-10-8-7-9-11-14)13-17(18(16)21)20(4,5)6/h7-
InchiKey: JIEWQZNTUPWNMX-UHFFFAOYSA-N
Formula: C20H26O
SMILES: CC(C)(C)c1cc(-c2ccccc2)cc(C(C)(C)C)c1O
Mol. weight [g/mol]: 282.42
CAS: 2668-47-5

Physical Properties

Property code	Value	Unit	Source
chs	-11280.00	kJ/mol	NIST Webbook
gf	174.14	kJ/mol	Joback Method
hf	-156.80	kJ/mol	NIST Webbook
hfs	-300.00	kJ/mol	NIST Webbook
hfus	25.82	kJ/mol	Joback Method
hsub	144.40	kJ/mol	NIST Webbook
hsub	143.20	kJ/mol	NIST Webbook
hvap	76.41	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.654		Crippen Method
mcvol	251.010	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
tb	794.48	K	Joback Method
tc	1041.03	K	Joback Method
tf	509.60	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.09	J/mol×K	794.48	Joback Method
cpg	833.35	J/mol×K	999.94	Joback Method
cpg	818.26	J/mol×K	958.85	Joback Method

cpg	802.70	J/mol×K	917.75	Joback Method
cpg	786.46	J/mol×K	876.66	Joback Method
cpg	769.33	J/mol×K	835.57	Joback Method
cpg	848.17	J/mol×K	1041.03	Joback Method
dvisc	0.0000039	Pa×s	794.48	Joback Method
dvisc	0.0000060	Pa×s	747.00	Joback Method
dvisc	0.0000095	Pa×s	699.52	Joback Method
dvisc	0.0000163	Pa×s	652.04	Joback Method
dvisc	0.0000303	Pa×s	604.56	Joback Method
dvisc	0.0000626	Pa×s	557.08	Joback Method
dvisc	0.0001482	Pa×s	509.60	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=C2668475&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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