[1,1'-Biphenyl]-2-ol, 3-(1,1-dimethylethyl)-

Other names: 2-Biphenylol, 3-tert-butyl-
2-tert-Butyl-6-Phenylphenol
Phenol, 2-tert-butyl-6-phenyl-
3-Tert-butyl[1,1'-biphenyl]-2-ol
3-(1,1-dimethylethyl)[1,1'-biphenyl]-2-ol
Inchi: InChI=1S/C16H18O/c1-16(2,3)14-11-7-10-13(15(14)17)12-8-5-4-6-9-12/h4-11,17H,1-3H
InchiKey: HXVMQDBXJZKLEV-UHFFFAOYSA-N
Formula: C16H18O
SMILES: CC(C)(C)c1cccc(-c2ccccc2)c1O
Mol. weight [g/mol]: 226.31
CAS: 2416-98-0

Physical Properties

Property code	Value	Unit	Source
chl	-8704.40	kJ/mol	NIST Webbook
gf	147.25	kJ/mol	Joback Method
hf	-57.03	kJ/mol	NIST Webbook
hfl	-164.00	kJ/mol	NIST Webbook
hfus	23.26	kJ/mol	Joback Method
hvap	107.20	kJ/mol	NIST Webbook
hvap	107.00	kJ/mol	NIST Webbook
log10ws	-4.94		Crippen Method
logp	4.357		Crippen Method
mcvol	194.650	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
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
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

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=C2416980&Units=SI

Legend

chl: Standard liquid 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
hfl: Liquid phase 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