

2,2'-Biphenol, 3,3',5,5'-tetrakis(1,1-dimethylethyl)-

Inchi: InChI=1S/C28H42O2/c1-25(2,3)17-13-19(23(29)21(15-17)27(7,8)9)20-14-18(26(4,5)6)16

InchiKey: GDGDLBOVIAWEAD-UHFFFAOYSA-N

Formula: C28H42O2

SMILES: CC(C)(C)c1cc(-c2cc(C(C)(C)C)cc(C(C)(C)C)c2O)c(O)c(C(C)(C)C)c1

Mol. weight [g/mol]: 410.63

CAS: 6390-69-8

Physical Properties

Property code	Value	Unit	Source
gf	73.30	kJ/mol	Joback Method
hf	-583.69	kJ/mol	Joback Method
hfus	36.71	kJ/mol	Joback Method
hvap	105.97	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	7.955		Crippen Method
mcvol	369.600	ml/mol	McGowan Method
pc	1164.84	kPa	Joback Method
tb	1061.64	K	Joback Method
tc	1313.15	K	Joback Method
tf	741.36	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1300.97	J/mol×K	1061.64	Joback Method
cpg	1325.72	J/mol×K	1103.56	Joback Method
cpg	1351.33	J/mol×K	1145.48	Joback Method
cpg	1378.17	J/mol×K	1187.39	Joback Method
cpg	1406.60	J/mol×K	1229.31	Joback Method
cpg	1436.98	J/mol×K	1271.23	Joback Method
cpg	1469.69	J/mol×K	1313.15	Joback Method
dvisc	0.0000004	Pa×s	741.36	Joback Method
dvisc	0.0000002	Pa×s	794.74	Joback Method

dvisc	7.9097424e-08	Pa×s	848.12	Joback Method
dvisc	4.2800391e-08	Pa×s	901.50	Joback Method
dvisc	2.4805790e-08	Pa×s	954.88	Joback Method
dvisc	1.5231479e-08	Pa×s	1008.26	Joback Method
dvisc	9.8227049e-09	Pa×s	1061.64	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=C6390698&Units=SI

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

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