

3,3',4,4'-Biphenyltetrol

Other names:	3,3',4,4'-Tetrahydroxydiphenyl 1,1'-Biphenyl-3,3',4,4'-tetrol
Inchi:	InChI=1S/C12H10O4/c13-9-3-1-7(5-11(9)15)8-2-4-10(14)12(16)6-8/h1-6,13-16H
InchiKey:	MZEFNGQKJROKHS-UHFFFAOYSA-N
Formula:	C12H10O4
SMILES:	Oc1ccc(-c2ccc(O)c(O)c2)cc1O
Mol. weight [g/mol]:	218.21
CAS:	3598-30-9

Physical Properties

Property code	Value	Unit	Source
gf	-343.50	kJ/mol	Joback Method
hf	-527.19	kJ/mol	Joback Method
hfus	38.05	kJ/mol	Joback Method
hvap	98.91	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.176		Crippen Method
mvol	155.900	ml/mol	McGowan Method
pc	8087.06	kPa	Joback Method
tb	849.80	K	Joback Method
tc	1127.72	K	Joback Method
tf	724.72	K	Joback Method
vc	0.355	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.87	J/molxK	849.80	Joback Method
cpg	462.07	J/molxK	896.12	Joback Method
cpg	474.16	J/molxK	942.44	Joback Method
cpg	487.55	J/molxK	988.76	Joback Method
cpg	502.68	J/molxK	1035.08	Joback Method
cpg	519.97	J/molxK	1081.40	Joback Method
cpg	539.85	J/molxK	1127.72	Joback Method

dvisc	1.7450781e-08	Paxs	724.72	Joback Method
dvisc	1.1172398e-08	Paxs	745.57	Joback Method
dvisc	7.3284750e-09	Paxs	766.41	Joback Method
dvisc	4.9156340e-09	Paxs	787.26	Joback Method
dvisc	3.3658411e-09	Paxs	808.11	Joback Method
dvisc	2.3489875e-09	Paxs	828.95	Joback Method
dvisc	1.6685223e-09	Paxs	849.80	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=C3598309&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
mvol:	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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