3,4-Hexanediol, 3,4-bis(4-hydroxyphenyl)-

Other names:	3,4-Bis(p-hydroxyphenyl)-3,4-hexanediol
	«alpha»,«alpha»'-Dihydroxydiethylstilbestrol
	3,4-Hexanediol, 3,4-bis(p-hydroxyphenyl)-
	3,4-bis(4-hydroxyphenyl)hexane-3,4-diol
Inchi:	InChI=1S/C18H22O4/c1-3-17(21,13-5-9-15(19)10-6-13)18(22,4-2)14-7-11-16(20)12-8-14
InchiKey:	MOGCNGHSEICQCE-UHFFFAOYSA-N
Formula:	C18H22O4
SMILES:	CCC(O)(c1ccc(O)cc1)C(O)(CC)c1ccc(O)cc1
Mol. weight [g/mol]:	302.36
CAS:	7507-01-9

Physical Properties

Property code	Value	Unit	Source
gf	-251.70	kJ/mol	Joback Method
hf	-618.37	kJ/mol	Joback Method
hfus	35.37	kJ/mol	Joback Method
hvap	117.01	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.993		Crippen Method
mcvol	240.440	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	1003.74	K	Joback Method
tc	1239.59	K	Joback Method
tf	695.38	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.40	J/mol×K	1003.74	Joback Method
cpg	812.05	J/mol×K	1043.05	Joback Method
cpg	827.33	J/mol×K	1082.36	Joback Method
cpg	843.48	J/mol×K	1121.67	Joback Method
cpg	860.77	J/mol×K	1160.98	Joback Method

cpg	879.44	J/mol×K	1200.28	Joback Method
cpg	899.73	J/mol×K	1239.59	Joback Method
dvisc	0.0000002	Pa×s	695.38	Joback Method
dvisc	5.7687052e-08	Pa×s	746.77	Joback Method
dvisc	2.2309814e-08	Pa×s	798.17	Joback Method
dvisc	9.6790143e-09	Pa×s	849.56	Joback Method
dvisc	4.6189312e-09	Pa×s	900.95	Joback Method
dvisc	2.3874188e-09	Pa×s	952.35	Joback Method
dvisc	1.3202796e-09	Pa×s	1003.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7507019&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

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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