Hexestrol

Other names:

(R*,S*)-4,4'-(1,2-diethyl-1,2-ethanediyl)bisphenol
(R*,S*)-4,4'-(1,2-diethylethylene)bis(phenol)
3,4-Bis(p-hydroxyphenyl)hexane
4,4'-(1,2-Diethylethylene)bis(phenol), (R*,S*)-
4,4'-Dihydroxy-«alpha»,«beta»-diethyldiphenylethane, meso
4,4'-Dihydroxy-«gamma»,«delta»-diphenylhexane, meso
4,4'-Dihydroxy-Â«alphaÂ»,Â«betaÂ»-diethyldiphenylethane, meso
4,4'-Dihydroxy-Â«gammaÂ»,Â«deltaÂ»-diphenylhexane, meso
Bibenzyl, «alpha»,«alpha»'-diethyl-4,4'-dihydroxy-
Bibenzyl, Â«alphaÂ»,Â«alphaÂ»'-diethyl-4,4'-dihydroxy-
Cycloestrol
Dihydrodiethylstilbestrol, meso
Dihydrostilbestrol, meso
Erythrohexestrol
Estra-Plex
Estrifar
Estronal
Extra-Plex
Hexane, 3,4-bis(p-hydroxyphenyl)-, meso
Hexanoestrol
Hexestrofen
Hexoestrol
Hexron
Hormoestrol
NSC-9894
Phenol, 4,4'-(1,2-diethyl-1,2-ethanediyl)bis-, (R*,S*)-
Phenol, 4,4'-(1,2-diethyl-1,2-ethylenediyl)bis-, (R*,S*)-
Phenol, 4,4'-(1,2-diethylethylene)di-, meso-
Sinestrol
Stilbestrol, dihydro-
Synestrol
Synoestrol
Synthovo
Syntrogene
meso-3,4-Bis(p-hydroxyphenyl)-n-hexane
meso-3,4-Di(p-hydroxyphenyl)-n-hexane
meso-Hexestrol
meso-Vitestrol
«gamma»,«delta»-Di(p-hydroxyphenyl)-hexane, meso
Â«gammaÂ»,Â«deltaÂ»-Di(p-hydroxyphenyl)-hexane, meso

Inchi: InChI=1S/C18H22O2/c1-3-17(13-5-9-15(19)10-6-13)18(4-2)14-7-11-16(20)12-8-14/h5-12
InchiKey: PBBGSZCBWVPOOL-ZENAZSQFSA-N
Formula: C18H22O2
SMILES: CCC(c1ccc(O)cc1)C(CC)c1ccc(O)cc1
Mol. weight [g/mol]: 270.37
CAS: 84-16-2

Physical Properties

Property code	Value	Unit	Source
gf	11.38	kJ/mol	Joback Method
hf	-306.97	kJ/mol	Joback Method
hfus	34.98	kJ/mol	Joback Method
hvap	85.47	kJ/mol	Joback Method
log10ws	-4.43		Estimated Solubility Method
log10ws	-4.43		Aqueous Solubility Prediction Method
logp	4.785		Crippen Method
mcvol	228.700	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	2402.00		NIST Webbook
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
rinpol	2402.00		NIST Webbook
tb	824.96	K	Joback Method
tc	1069.32	K	Joback Method
tf	459.65	K	Aqueous Solubility Prediction Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.53	J/mol×K	824.96	Joback Method
cpg	707.49	J/mol×K	865.69	Joback Method
cpg	722.82	J/mol×K	906.41	Joback Method
cpg	737.74	J/mol×K	947.14	Joback Method
cpg	752.46	J/mol×K	987.87	Joback Method

cpg	767.18	J/mol×K	1028.59	Joback Method
cpg	782.12	J/mol×K	1069.32	Joback Method
dvisc	0.0000320	Pa×s	538.90	Joback Method
dvisc	0.0000109	Pa×s	586.58	Joback Method
dvisc	0.0000043	Pa×s	634.25	Joback Method
dvisc	0.0000020	Pa×s	681.93	Joback Method
dvisc	0.0000010	Pa×s	729.61	Joback Method
dvisc	0.0000005	Pa×s	777.28	Joback Method
dvisc	0.0000003	Pa×s	824.96	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C84162&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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