Diethylstilbestrol

Other names:

(E)-3,4-Bis(4-hydroxyphenyl)-3-hexene
(E)-4,4'-(1,2-Diethyl-1,2-ethenediyl)bisphenol
3,4-(Di-4-hydroxyphenyl)hex-3-ene, (E)-
3,4-Bis(p-hydroxyphenyl)-3-hexene, trans
3-Hexene,3,4-bis(p-hydroxyphenyl)-, (E)-
4,4'-(1,2-Diethyl-1,2-ethenediyl)bisphenol, trans
4,4'-Dihydroxy-«alpha»,«beta»-diethylstilbene
4,4'-Dihydroxy-Â«alphaÂ»,Â«betaÂ»-diethylstilbene
4,4'-Dihydroxydiethylstilbene
4,4'-Stilbenediol, «alpha»,«alpha»'-diethyl-, (E)-
4,4'-Stilbenediol, «alpha»,«alpha»-diethyl-, (E)-
4,4'-Stilbenediol, Â«alphaÂ»,Â«alphaÂ»'-diethyl-, (E)-
4,4'-Stilbenediol, Â«alphaÂ»,Â«alphaÂ»-diethyl-, (E)-
Acnestrol
Agostilben
Antigestil
Bertrol
Bio-des
Bufon
Climaterine
Comestrol
Comestrol estrobene
Cyren
Cyren A
DEB
DES
DES (Synthetic Estrogen)
Dawe's destrol
Desma
Destrol
Di-Estryl
DiBestrol 2 Premix
Diastyl
Dibestrol
Dibestrol '2' premix
Dicorvin
Diethylstilbesterol
Diethylstilboesterol
Dietilestilbestrol
Distilbene

Domestrol
Dyestrol
Estilben
Estilbin MCO
Estril
Estrobene
Estromenin
Estrosyn
Follidiene
Fonatol
Grafestrol
Gynopharm
Hi-Bestrol
Idroestril
Iscovesco
Makarol
Menostilbeen
Micrest
Microest
Milestrol
NSC 3070
Neo-Oestranol I
New-Estranol 1
OeKolp
Oestrogenine
Oestrol vetag
Oestromenin
Oestromensil
Oestromensyl
Oestromienin
Oestromon
Pabestrol
Palestrol
Percutatrine oestrogenique iscovesco
Phenol, 4,4'-(1,2-diethyl-1,2-ethenediyl)bis-, (E)-
Phenol, 4,4'-[(1E)-1,2-diethyl-1,2-ethenediyl]bis-
Protectona
RCRA Waste number U089
Rumestrol 1
Rumestrol 2
Sedestran
Serral
Sexocretin

Sibol
Sintestrol
Stibilium
Stil
Stil-Rol
Stilbestrol
Stilbestrol, diethyl-
Stilbestrone
Stilbetin
Stilboefral
Stilboestroform
Stilboestrol
Stilbofolin
Stilbol
Stilkap
Synestrin
Synthestrin
Synthoestrin
Synthofolin
Syntofolin
Tampovagan stilboestrol
Tylosterone
Vagestrol
neo-Oestranol 1
strobene
trans-4,4'-(1,2-Diethyl-1,2-ethenediyl)bisphenol
trans-Diethylstilbesterol
trans-Diethylstilbestrol
trans-Diethylstilboesterol
trans-«alpha»,«alpha»'-Diethyl-4,4'-Stilbenediol
trans-Â«alphaÂ»,Â«alphaÂ»'-Diethyl-4,4'-Stilbenediol
«alpha»,«alpha»'-Diethyl-(E)-4,4'-stilbenediol
«alpha»,«alpha»'-Diethyl-4,4'-stilbenediol
«alpha»,«alpha»'-Diethylstilbenediol
Â«alphaÂ»,Â«alphaÂ»'-Diethyl-(E)-4,4'-stilbenediol
Â«alphaÂ»,Â«alphaÂ»'-Diethyl-4,4'-stilbenediol
Â«alphaÂ»,Â«alphaÂ»'-Diethylstilbenediol

Inchi: InChI=1S/C18H20O2/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: RGLYKWWBQGJZGM-ISLYRVAYSA-N

Formula: C18H20O2

SMILES: CCC(=C(CC)c1ccc(O)cc1)c1ccc(O)cc1

Mol. weight [g/mol]: 268.35

CAS: 56-53-1

Physical Properties

Property code	Value	Unit	Source
gf	79.38	kJ/mol	Joback Method
hf	-198.77	kJ/mol	Joback Method
hfus	39.61	kJ/mol	Joback Method
hvap	86.36	kJ/mol	Joback Method
log10ws	-4.19		Aqueous Solubility Prediction Method
log10ws	-4.07		Estimated Solubility Method
logp	4.829		Crippen Method
mcvol	224.400	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	2298.00		NIST Webbook
tb	829.76	K	Joback Method
tc	1081.28	K	Joback Method
tf	445.56 ± 0.20	K	NIST Webbook
tf	443.00 ± 1.00	K	NIST Webbook
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.01	J/mol×K	1039.36	Joback Method
cpg	663.14	J/mol×K	829.76	Joback Method
cpg	678.69	J/mol×K	871.68	Joback Method
cpg	693.80	J/mol×K	913.60	Joback Method
cpg	708.72	J/mol×K	955.52	Joback Method
cpg	723.71	J/mol×K	997.44	Joback Method
cpg	754.89	J/mol×K	1081.28	Joback Method
hfust	31.76	kJ/mol	443.80	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56531&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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