

Estriol, trimethyl ether

Other names:	(16«alpha»,17«beta»)-3,16,17-Trimethoxyestra-1(10),2,4-triene
Inchi:	InChI=1S/C21H30O3/c1-21-10-9-16-15-8-6-14(22-2)11-13(15)5-7-17(16)18(21)12-19(23)
InchiKey:	QIOWNWWZXNWWMP-UHFFFAOYSA-N
Formula:	C21H30O3
SMILES:	COc1ccc2c(c1)CCC1C2CCC2(C)C1CC(OC)C2OC
Mol. weight [g/mol]:	330.46

Physical Properties

Property code	Value	Unit	Source
gf	33.52	kJ/mol	Joback Method
hf	-499.54	kJ/mol	Joback Method
hfus	34.09	kJ/mol	Joback Method
hvap	71.17	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.191		Crippen Method
mvol	268.020	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	2698.20		NIST Webbook
tb	798.77	K	Joback Method
tc	1024.65	K	Joback Method
tf	502.54	K	Joback Method
vc	1.008	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.83	J/molxK	798.77	Joback Method
cpg	912.14	J/molxK	836.42	Joback Method
cpg	934.44	J/molxK	874.06	Joback Method
cpg	955.88	J/molxK	911.71	Joback Method
cpg	976.62	J/molxK	949.35	Joback Method
cpg	996.83	J/molxK	987.00	Joback Method
cpg	1016.66	J/molxK	1024.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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