

Estra-1,3,5(10)-trien-3-ol, 16,17-epoxy-, (16«beta»,17«beta»)-

Other names:1,3,5(10)-Oestratrien-3-ol, 16«beta»,17«beta»-epoxy, TFA

Inchi:InChI=1S/C18H22O2/c1-18-7-6-13-12-5-3-11(19)8-10(12)2-4-14(13)15(18)9-16-17(18)20

InchiKey:XPXOJYZDBJGFEI-UHFFFAOYSA-N

Formula:C18H22O2

SMILES:CC12CCC3c4ccc(O)cc4CCC3C1CC1OC12

Mol. weight [g/mol]:270.37

CAS:472-57-1

Physical Properties

Property code	Value	Unit	Source
gf	184.81	kJ/mol	Joback Method
hf	-233.34	kJ/mol	Joback Method
hfus	38.17	kJ/mol	Joback Method
hvap	74.01	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.626		Crippen Method
mcvol	209.020	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	2330.00		NIST Webbook
tb	768.33	K	Joback Method
tc	1019.88	K	Joback Method
tf	557.03	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.05	J/mol×K	768.33	Joback Method
cpg	714.43	J/mol×K	810.26	Joback Method
cpg	734.42	J/mol×K	852.18	Joback Method
cpg	754.42	J/mol×K	894.11	Joback Method
cpg	774.88	J/mol×K	936.03	Joback Method
cpg	796.22	J/mol×K	977.96	Joback Method
cpg	818.87	J/mol×K	1019.88	Joback Method

Sources

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=C472571&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
hvac:	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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