

Estra-1,3,5(10)-triene-16beta-yiacetic acid lactone, 17beta-hydroxy-3-methoxy-

Inchi:	InChI=1S/C21H26O3/c1-21-8-7-16-15-6-4-14(23-2)9-12(15)3-5-17(16)18(21)10-13-11-19
InchiKey:	BMTIHQRYKLLCCZ-UHFFFAOYSA-N
Formula:	C21H26O3
SMILES:	COc1ccc2c(c1)CCC1C2CCC2(C)C1CC1CC(=O)OC12
Mol. weight [g/mol]:	326.43
CAS:	95282-75-0

Physical Properties

Property code	Value	Unit	Source
gf	103.27	kJ/mol	Joback Method
hf	-411.66	kJ/mol	Joback Method
hfus	36.27	kJ/mol	Joback Method
hvap	75.33	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.093		Crippen Method
mcvol	252.860	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
tb	860.11	K	Joback Method
tc	1111.08	K	Joback Method
tf	575.05	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.89	J/molxK	860.11	Joback Method
cpg	906.10	J/molxK	901.94	Joback Method
cpg	928.66	J/molxK	943.77	Joback Method
cpg	950.84	J/molxK	985.59	Joback Method
cpg	972.90	J/molxK	1027.42	Joback Method
cpg	995.12	J/molxK	1069.25	Joback Method
cpg	1017.77	J/molxK	1111.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95282750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
mccol:	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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