

5-Pregnen-3beta-ol, 16alpha,17alpha-epoxy-20-ethylenedioxy-, acetate

InChI:	InChI=1S/C25H36O5/c1-15(26)29-17-7-9-22(2)16(13-17)5-6-18-19(22)8-10-23(3)20(18)
InChIKey:	DXUKESFRWHAYGS-UHFFFAOYSA-N
Formula:	C25H36O5
SMILES:	CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C3CC3OC32C2(C)OCCO2)C1
Mol. weight [g/mol]:	416.55
CAS:	27255-57-8

Physical Properties

Property code	Value	Unit	Source
gf	-53.42	kJ/mol	Joback Method
hf	-747.88	kJ/mol	Joback Method
hfus	44.39	kJ/mol	Joback Method
hvap	89.69	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.391		Crippen Method
mcvol	318.700	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
tb	981.42	K	Joback Method
tc	1236.32	K	Joback Method
tf	709.58	K	Joback Method
vc	1.200	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1258.86	J/molxK	981.42	Joback Method
cpg	1302.46	J/molxK	1023.90	Joback Method
cpg	1350.30	J/molxK	1066.39	Joback Method
cpg	1403.17	J/molxK	1108.87	Joback Method
cpg	1461.86	J/molxK	1151.35	Joback Method
cpg	1527.18	J/molxK	1193.84	Joback Method
cpg	1599.92	J/molxK	1236.32	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27255578&Units=SI

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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