

5,16-Pregnenolone oxime

Other names:	Pregn-5,16-dienolone 20-oxime Pregna-5,16-diene-20-one oxime, 3«beta»-hydroxy Pregna-5,16-dien-20-one, 3-hydroxy-, oxime, (3«beta»)- Pregna-5,16-diene-20-one oxime, 3beta-hydroxy
Inchi:	InChI=1S/C21H31NO2/c1-13(22-24)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9
InchiKey:	PUAYLIXQYVQBPE-UHFFFAOYSA-N
Formula:	C21H31NO2
SMILES:	CC(=NO)C1=CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	329.48
CAS:	1045-71-2

Physical Properties

Property code	Value	Unit	Source
hf	-365.98	kJ/mol	Joback Method
hvap	98.59	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.697		Crippen Method
mvol	272.130	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
tb	988.53	K	Joback Method
tc	1220.43	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1045712&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

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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