

Allopregnan-3«alpha»-ol-20-one

Other names:

Pregnan-20-one, 3-hydroxy-, (3«alpha»,5«alpha»)-
5«alpha»-Pregnan-20-one, 3«alpha»-hydroxy-
3-«alpha»-Hydroxy-5-«alpha»-pregnan-20-one
Allopregnan-3«beta»-ol-20-one
Allopregnanolone

Inchi:

InChI=1S/C21H34O2/c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-2

InchiKey:

AURFZBICLPNKBZ-QPSUBATNSA-N

Formula:

C₂₁H₃₄O₂

SMILES:

CC(=O)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C

Mol. weight [g/mol]:

318.49

CAS:

516-54-1

Physical Properties

Property code	Value	Unit	Source
gf	0.88	kJ/mol	Joback Method
hf	-532.06	kJ/mol	Joback Method
hfus	29.56	kJ/mol	Joback Method
hvap	82.74	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.595		Crippen Method
mcvol	270.750	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
tb	856.04	K	Joback Method
tc	1080.43	K	Joback Method
tf	467.00 ± 8.00	K	NIST Webbook
tf	409.00 ± 5.00	K	NIST Webbook
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.31	J/mol×K	856.04	Joback Method
cpg	1006.66	J/mol×K	893.44	Joback Method
cpg	1031.94	J/mol×K	930.84	Joback Method

cpg	1057.47	J/mol×K	968.24	Joback Method
cpg	1083.54	J/mol×K	1005.63	Joback Method
cpg	1110.47	J/mol×K	1043.03	Joback Method
cpg	1138.56	J/mol×K	1080.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C516541&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvap:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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