

Pregnan-3«alpha»-ol-20-one

Other names:	Pregnan-20-one, 3-hydroxy-, (3«alpha»,5«beta»)- 5«beta»-Pregnan-20-one, 3«alpha»-hydroxy- Pregnanolone II SKF 6455 3«alpha»-Hydroxy-5«beta»-tetrahydroprogesterone 3«alpha»,5«beta»-Epimeric pregnanolone 3«alpha»-Hydroxy-5«beta»-pregnan-20-one Pregnanolone 3«alpha»,5«beta»-Pregnanolone 3-Hydroxypregnan-20-one, (3«alpha»,5«beta»)- 3alpha-hydroxy-5beta-Pregnan-20-one 5beta-Pregnan-3alpha-ol-20-one 5«beta»-Pregnan-3«alpha»-ol-20-one NSC 82867 5B-Pregnan-3A-ol-20-one
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-ZGLJFNAKSA-N
Formula:	C21H34O2
SMILES:	CC(=O)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	318.49
CAS:	128-20-1

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
rinpol	2642.00		NIST Webbook
rinpol	2643.00		NIST Webbook
rinpol	2605.00		NIST Webbook
tb	856.04	K	Joback Method
tc	1080.43	K	Joback Method

tf	522.18	K	Joback Method
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

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=C128201&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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