

Pregnenolone acetate

Other names:	Pregn-5-en-20-one, 3-(acetyloxy)-, (3«beta»)- Pregn-5-en-20-one, 3«beta»-hydroxy-, acetate Antofin Artivis Enescorb Pregenolone acetate Pregnenolone-3-acetate Previsone Sharmone 5-Pregnen-3-«beta»-ol-20-one acetate 20-Oxopregn-5-en-3«beta»-yl acetate 5-Allopregnene-3«beta»-ol-20-one acetate 5-Pregnenolone acetate 3«beta»-Acetoxypregn-5-en-20-one 3Beta-acetoxypregn-5-en-20-one
Inchi:	InChI=1S/C23H34O3/c1-14(24)19-7-8-20-18-6-5-16-13-17(26-15(2)25)9-11-22(16,3)21(1
InchiKey:	CRRKVZVYZQXICQ-AKCLOJTASA-N
Formula:	C23H34O3
SMILES:	CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)=O)CCC32)C1
Mol. weight [g/mol]:	358.51
CAS:	1778-02-5

Physical Properties

Property code	Value	Unit	Source
gf	-51.34	kJ/mol	Joback Method
hf	-599.26	kJ/mol	Joback Method
hfus	33.20	kJ/mol	Joback Method
hvap	80.93	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	5.086		Crippen Method
mvol	296.200	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
tb	894.72	K	Joback Method
tc	1131.47	K	Joback Method
tf	573.58	K	Joback Method
vc	1.121	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.02	J/mol×K	894.72	Joback Method
cpg	1085.02	J/mol×K	934.18	Joback Method
cpg	1112.19	J/mol×K	973.64	Joback Method
cpg	1139.86	J/mol×K	1013.10	Joback Method
cpg	1168.39	J/mol×K	1052.56	Joback Method
cpg	1198.11	J/mol×K	1092.01	Joback Method
cpg	1229.37	J/mol×K	1131.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1778025&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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