

5Beta-hydroxycholestan-3-one

Inchi:	InChI=1S/C27H46O2/c1-18(2)7-6-8-19(3)22-9-10-23-21-12-16-27(29)17-20(28)11-15-26
InchiKey:	OPSNLRNZVIABPI-UHFFFAOYSA-N
Formula:	C27H46O2
SMILES:	CC(C)CCCC(C)C1CCC2C3CCC4(O)CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	402.65
CAS:	19043-70-0

Physical Properties

Property code	Value	Unit	Source
gf	55.07	kJ/mol	Joback Method
hf	-656.00	kJ/mol	Joback Method
hfus	28.60	kJ/mol	Joback Method
hvap	91.98	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.792		Crippen Method
mcvol	355.290	ml/mol	McGowan Method
pc	1121.55	kPa	Joback Method
tb	1011.30	K	Joback Method
tc	1245.29	K	Joback Method
tf	606.23	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1411.78	J/molxK	1011.30	Joback Method
cpg	1450.15	J/molxK	1050.30	Joback Method
cpg	1490.53	J/molxK	1089.30	Joback Method
cpg	1533.37	J/molxK	1128.29	Joback Method
cpg	1579.12	J/molxK	1167.29	Joback Method
cpg	1628.24	J/molxK	1206.29	Joback Method
cpg	1681.16	J/molxK	1245.29	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=C19043700&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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