

Cholesta-8,14-dien-3-ol, (3«beta»,5«alpha»)-

Other names:	5«alpha»-Cholesta-8,14-dien-3«beta»-ol «delta»8,14-Cholestadienol 5«alpha»-Cholesta-8,14-diene-3«beta»-ol
Inchi:	InChI=1S/C27H44O/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(28)13-15-26(20,4
InchiKey:	AWBZPJQUWZBRII-BDHCHTMKSA-N
Formula:	C27H44O
SMILES:	CC(C)CCCC(C)C1CC=C2C3=C(CCC21C)C1(C)CCC(O)CC1CC3
Mol. weight [g/mol]:	384.64
CAS:	19431-20-0

Physical Properties

Property code	Value	Unit	Source
gf	229.60	kJ/mol	Joback Method
hf	-411.71	kJ/mol	Joback Method
hfus	34.52	kJ/mol	Joback Method
hvap	92.07	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	7.453		Crippen Method
mcvol	345.120	ml/mol	McGowan Method
pc	1131.38	kPa	Joback Method
rinpol	3135.00		NIST Webbook
tb	965.84	K	Joback Method
tc	1190.08	K	Joback Method
tf	561.67	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.97	J/mol×K	965.84	Joback Method
cpg	1312.09	J/mol×K	1003.21	Joback Method
cpg	1343.05	J/mol×K	1040.59	Joback Method
cpg	1375.18	J/mol×K	1077.96	Joback Method
cpg	1408.82	J/mol×K	1115.33	Joback Method

cpg	1444.31	J/mol×K	1152.70	Joback Method
cpg	1481.97	J/mol×K	1190.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19431200&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

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
hvac:	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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