

Cholest-7-en-3-ol, 4-methyl-, (3«beta»,4«alpha»,5«alpha»)-

Other names:	4-«alpha»-Methyl-5-«alpha»-cholest-7-en-3-«beta»-ol
Inchi:	InChI=1S/C28H48O/c1-18(2)8-7-9-19(3)22-12-13-24-21-10-11-23-20(4)26(29)15-17-28(2)
InchiKey:	LMYZQUNLYGJIHI-GQDVSBTQSA-N
Formula:	C28H48O
SMILES:	CC(C)CCCC(C)C1CCC2C3=CCC4C(C)C(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	400.68
CAS:	481-25-4

Physical Properties

Property code	Value	Unit	Source
gf	204.19	kJ/mol	Joback Method
hf	-528.21	kJ/mol	Joback Method
hfus	39.88	kJ/mol	Joback Method
hvap	91.75	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	7.635		Crippen Method
mcvol	363.510	ml/mol	McGowan Method
pc	992.63	kPa	Joback Method
rinpol	3225.00		NIST Webbook
rinpol	3225.00		NIST Webbook
tb	965.59	K	Joback Method
tc	1187.42	K	Joback Method
tf	534.42	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1389.24	J/molxK	965.59	Joback Method
cpg	1420.61	J/molxK	1002.56	Joback Method
cpg	1452.48	J/molxK	1039.53	Joback Method
cpg	1485.16	J/molxK	1076.51	Joback Method
cpg	1518.98	J/molxK	1113.48	Joback Method
cpg	1554.23	J/molxK	1150.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C481254&Units=SI

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
mccvol:	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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