

Cholest-5-en-3-ol, 4,4-dimethyl-, (3«beta»)-

Other names:	Cholest-5-en-3«beta»-ol, 4,4-dimethyl- 4,4-Dimethylcholest-5-enol 4,4-Dimethylcholesterol 4,4-Dimethylcholest-5-en-3-«beta»-ol
Inchi:	InChI=1S/C29H50O/c1-19(2)9-8-10-20(3)22-12-13-23-21-11-14-25-27(4,5)26(30)16-18-2
InchiKey:	DASOUCLGLBPXLC-UTYNOFFGSA-N
Formula:	C29H50O
SMILES:	<chem>CC(C)CCCC(C)C1CCC2C3CC=C4C(C)(C)C(O)CCC4(C)C3CCC12C</chem>
Mol. weight [g/mol]:	414.71
CAS:	1253-88-9

Physical Properties

Property code	Value	Unit	Source
gf	207.12	kJ/mol	Joback Method
hf	-533.61	kJ/mol	Joback Method
hfus	36.17	kJ/mol	Joback Method
hvap	92.83	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	8.025		Crippen Method
mcvol	377.600	ml/mol	McGowan Method
pc	961.48	kPa	Joback Method
rinpol	3260.00		NIST Webbook
rinpol	3260.00		NIST Webbook
tb	988.71	K	Joback Method
tc	1214.81	K	Joback Method
tf	569.59	K	Joback Method
vc	1.431	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1466.17	J/mol×K	988.71	Joback Method
cpg	1504.00	J/mol×K	1026.39	Joback Method
cpg	1543.61	J/mol×K	1064.08	Joback Method

cpg	1585.43	J/mol×K	1101.76	Joback Method
cpg	1629.88	J/mol×K	1139.44	Joback Method
cpg	1677.41	J/mol×K	1177.13	Joback Method
cpg	1728.44	J/mol×K	1214.81	Joback Method

Sources

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=C1253889&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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