

Cholestan-3-ol, 4,4-dimethyl-, (3«beta»,5«alpha»)-

Other names:

4,4-Dimethylcholestan-3-ol-, (3«beta»,5«alpha»)-

4,4-Dimethyl-5-«alpha»-cholestan-3-«beta»-ol

Inchi: InChI=1S/C29H52O/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: PCWHWFOTXAIVFT-WVYPIYABSA-N

Formula: C29H52O

SMILES: CC(C)CCCC(C)C1CCC2C3CCC4C(C)(C)C(O)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 416.72

CAS: 2550-84-7

Physical Properties

Property code	Value	Unit	Source
gf	179.08	kJ/mol	Joback Method
hf	-600.26	kJ/mol	Joback Method
hfus	36.41	kJ/mol	Joback Method
hvap	91.57	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	8.105		Crippen Method
mcvol	381.900	ml/mol	McGowan Method
pc	930.07	kPa	Joback Method
rinpol	3265.00		NIST Webbook
rinpol	3265.00		NIST Webbook
tb	979.90	K	Joback Method
tc	1204.03	K	Joback Method
tf	552.07	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1498.15	J/molxK	979.90	Joback Method
cpg	1535.98	J/molxK	1017.26	Joback Method
cpg	1575.30	J/molxK	1054.61	Joback Method
cpg	1616.56	J/molxK	1091.97	Joback Method
cpg	1660.16	J/molxK	1129.32	Joback Method

cpg	1706.52	J/mol×K	1166.68	Joback Method
cpg	1756.08	J/mol×K	1204.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2550847&Units=SI
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

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/74-636-4/Cholestan-3-ol-4-4-dimethyl-3-beta-5-alpha.pdf>

Generated by Cheméo on 2024-05-05 19:13:20.743629242 +0000 UTC m=+17225649.664206554.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.