

4,4,14-«alpha»-Trimethyl-5-«alpha»-cholestan-3-«alpha»-ol

Inchi: InChI=1S/C30H54O/c1-20(2)10-9-11-21(3)22-14-18-30(8)24-12-13-25-27(4,5)26(31)16-17
InchiKey: FPTJELQXIUUCEY-OOVRDAFLSA-N
Formula: C30H54O
SMILES: CC(C)CCCC(C)C1CCC2(C)C3CCC4C(C)(C)C(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 430.75

Physical Properties

Property code	Value	Unit	Source
gf	182.01	kJ/mol	Joback Method
hf	-605.66	kJ/mol	Joback Method
hfus	32.70	kJ/mol	Joback Method
hvap	92.64	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	8.495		Crippen Method
mvol	395.990	ml/mol	McGowan Method
pc	901.80	kPa	Joback Method
rinpol	3381.00		NIST Webbook
rinpol	3381.00		NIST Webbook
tb	1003.02	K	Joback Method
tc	1231.50	K	Joback Method
tf	587.24	K	Joback Method
vc	1.498	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1580.76	J/molxK	1003.02	Joback Method
cpg	1626.26	J/molxK	1041.10	Joback Method
cpg	1674.71	J/molxK	1079.18	Joback Method
cpg	1726.65	J/molxK	1117.26	Joback Method
cpg	1782.63	J/molxK	1155.34	Joback Method
cpg	1843.21	J/molxK	1193.42	Joback Method
cpg	1908.93	J/molxK	1231.50	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=R490523&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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