

Cholest-8-en-3-ol, 14-methyl-, (3«beta»,5«alpha»)-

Other names:	5«alpha»-Cholest-8-en-3«beta»-ol, 14-methyl-14«alpha»-Methyl-«delta»8-cholestenol 14«alpha»-methyl-5«alpha»-cholest-8(14)-en-3«beta»-ol 14-Methylcholest-8-en-3-ol, (3«beta»,5«alpha»)-
Inchi:	InChI=1S/C28H48O/c1-19(2)8-7-9-20(3)23-13-16-28(6)25-11-10-21-18-22(29)12-15-26(2)
InchiKey:	CYEADWAQMXQSDD-UHFFFAOYSA-N
Formula:	C28H48O
SMILES:	CC(C)CCCC(C)C1CCC2(C)C3=C(CCC12C)C1(C)CCC(O)CC1CC3
Mol. weight [g/mol]:	400.68
CAS:	6062-47-1

Physical Properties

Property code	Value	Unit	Source
gf	204.49	kJ/mol	Joback Method
hf	-483.76	kJ/mol	Joback Method
hfus	31.05	kJ/mol	Joback Method
hvap	91.88	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	7.923		Crippen Method
mcvol	363.510	ml/mol	McGowan Method
pc	1055.51	kPa	Joback Method
tb	980.15	K	Joback Method
tc	1206.51	K	Joback Method
tf	579.32	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1390.28	J/mol×K	980.15	Joback Method
cpg	1427.00	J/mol×K	1017.88	Joback Method
cpg	1465.61	J/mol×K	1055.60	Joback Method
cpg	1506.53	J/mol×K	1093.33	Joback Method
cpg	1550.21	J/mol×K	1131.06	Joback Method

cpg	1597.10	J/mol×K	1168.78	Joback Method
cpg	1647.63	J/mol×K	1206.51	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6062471&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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