24-Methyl-5-«alpha»-cholest-22-en-3-«beta»-ol

Inchi: InChI=1S/C28H48O/c1-18(2)19(3)7-8-20(4)24-11-12-25-23-10-9-21-17-22(29)13-15-27(2
InchiKey: PRKPDIRLXGMLSU-WGOAJHFPSA-N
Formula: C28H48O
SMILES: CC(C)C(C)C=CC(C)C1CCC2C3=CCC4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 400.68
CAS: 59905-70-3

Physical Properties

Property code	Value	Unit	Source
gf	289.68	kJ/mol	Joback Method
hf	-395.93	kJ/mol	Joback Method
hfus	35.49	kJ/mol	Joback Method
hvap	91.63	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	7.411		Crippen Method
mcvol	359.210	ml/mol	McGowan Method
pc	1053.46	kPa	Joback Method
rinpol	3220.00		NIST Webbook
rinpol	3220.00		NIST Webbook
tb	973.98	K	Joback Method
tc	1201.12	K	Joback Method
tf	518.58	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1359.87	J/mol×K	973.98	Joback Method
cpg	1391.77	J/mol×K	1011.84	Joback Method
cpg	1424.52	J/mol×K	1049.69	Joback Method
cpg	1458.49	J/mol×K	1087.55	Joback Method
cpg	1494.04	J/mol×K	1125.41	Joback Method
cpg	1531.52	J/mol×K	1163.26	Joback Method
cpg	1571.31	J/mol×K	1201.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59905703&Units=SI
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

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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