.GAMMA.-ergostenol

Other names: Ergost-7-en-3-ol, (3«beta»,5«alpha»)-
5«alpha»-Ergost-7-en-3«beta»-ol
«delta»7-Campestenol
«delta»7-Campesterol
Fungisterol
7-Ergostenol
24-Methyl-5-«alpha»-cholest-7-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: PUGBZUWUTZUUCP-CCAXXHQASA-N
Formula: C28H48O
SMILES: CC(C)C(C)CCC(C)C1CCC2C3=CC[C@H]4C[C@@H](O)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 400.69

Physical Properties

Property code	Value	Unit	Source
hfus	35.28	kJ/mol	Joback Method
logp	7.635		Crippen Method
mcvol	363.510	ml/mol	McGowan Method
rinpol	3220.00		NIST Webbook
rinpol	3220.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1386.76	J/mol×K	969.82	Joback Method
cpg	1418.35	J/mol×K	1007.10	Joback Method
cpg	1450.56	J/mol×K	1044.38	Joback Method
cpg	1483.71	J/mol×K	1081.65	Joback Method
cpg	1518.15	J/mol×K	1118.93	Joback Method
cpg	1554.19	J/mol×K	1156.21	Joback Method
cpg	1592.18	J/mol×K	1193.49	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C516789&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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