

Ergosta-5,24(28)-dien-3-ol, (3«beta»)-

Other names:	Ergosta-5,24(28)-dien-3«beta»-ol Chalinasterol Cholesterol, 24-methylene- Ostreasterol 24-Methylenecholesterol 24-Methylencholesterol
Inchi:	InChI=1S/C28H46O/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:	INDVLXYUCBVVKW-DMFCSKGGSA-N
Formula:	C28H46O
SMILES:	<chem>C=C(CCC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C)C(C)C</chem>
Mol. weight [g/mol]:	398.66
CAS:	474-63-5

Physical Properties

Property code	Value	Unit	Source
gf	291.19	kJ/mol	Joback Method
hf	-392.23	kJ/mol	Joback Method
hfus	36.22	kJ/mol	Joback Method
hvap	91.47	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	7.555		Crippen Method
mcvol	359.210	ml/mol	McGowan Method
pc	1044.62	kPa	Joback Method
rinpol	3117.00		NIST Webbook
rinpol	3133.00		NIST Webbook
rinpol	3108.00		NIST Webbook
rinpol	3108.00		NIST Webbook
rinpol	3135.00		NIST Webbook
rinpol	3155.00		NIST Webbook
rinpol	3155.00		NIST Webbook
rinpol	3108.00		NIST Webbook
rinpol	3135.00		NIST Webbook
rinpol	3136.00		NIST Webbook
rinpol	3108.00		NIST Webbook
rinpol	3121.00		NIST Webbook
rinpol	3095.00		NIST Webbook
rinpol	3135.00		NIST Webbook

rmpol	3117.00		NIST Webbook
tb	966.82	K	Joback Method
tc	1191.30	K	Joback Method
tf	522.94	K	Joback Method
vc	1.359	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1355.32	J/mol×K	966.82	Joback Method
cpg	1386.54	J/mol×K	1004.23	Joback Method
cpg	1418.47	J/mol×K	1041.65	Joback Method
cpg	1451.43	J/mol×K	1079.06	Joback Method
cpg	1485.78	J/mol×K	1116.48	Joback Method
cpg	1521.85	J/mol×K	1153.89	Joback Method
cpg	1559.99	J/mol×K	1191.30	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C474635&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
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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