Ergostanol

Other names:	Ergostan-3-ol, (3«beta»,5«alpha»)- 5«alpha»-Ergostan-3«beta»-ol Epiergostanol (3«beta»,5«alpha»)-Ergostan-3-ol 24S-Methyl-5-«alpha»-cholestan-3-«beta»-ol
Inchi:	InChI=1S/C28H50O/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:	ARYTXMNEANMLMU-KVOTZNMTSA-N
Formula:	C28H50O
SMILES:	CC(C)C(C)CCC(C)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	402.70
CAS:	6538-02-9

Physical Properties

Property code	Value	Unit	Source
gf	181.42	kJ/mol	Joback Method
hf	-579.80	kJ/mol	Joback Method
hfus	35.52	kJ/mol	Joback Method
hvap	90.41	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	7.715		Crippen Method
mcvol	367.810	ml/mol	McGowan Method
pc	984.55	kPa	Joback Method
rinpol	3210.00		NIST Webbook
rinpol	3210.00		NIST Webbook
tb	961.01	K	Joback Method
tc	1182.70	K	Joback Method
tf	506.14	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1419.59	J/mol×K	961.01	Joback Method
cpg	1451.53	J/mol×K	997.96	Joback Method

cpg	1483.87	J/mol×K	1034.91	Joback Method
cpg	1516.92	J/mol×K	1071.86	Joback Method
cpg	1551.02	J/mol×K	1108.80	Joback Method
cpg	1586.47	J/mol×K	1145.75	Joback Method
cpg	1623.61	J/mol×K	1182.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6538029&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