Ergost-8(14)-en-3-ol, (3«beta»)-

Other names:	Ergost-8(14)-en-3«beta»-ol 8(14)-Dehydro-hexahydroergosterol 3«beta»-Ergost-8(14)-en-3-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:	AWYDNKRGSOPYQB-AVPUWTLXSA-N
Formula:	C28H48O
SMILES:	CC(C)C(C)CCC(C)C1CCC2=C3CCC4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]:	400.68
CAS:	30365-65-2

Physical Properties

Property code	Value	Unit	Source
gf	207.54	kJ/mol	Joback Method
hf	-504.28	kJ/mol	Joback Method
hfus	33.82	kJ/mol	Joback Method
hvap	92.64	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	7.779		Crippen Method
mcvol	363.510	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	3215.00		NIST Webbook
rinpol	3215.00		NIST Webbook
tb	979.47	K	Joback Method
tc	1204.63	K	Joback Method
tf	540.42	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1385.21	J/mol×K	979.47	Joback Method
cpg	1417.14	J/mol×K	1017.00	Joback Method
cpg	1449.85	J/mol×K	1054.52	Joback Method
cpg	1483.68	J/mol×K	1092.05	Joback Method

cpg	1518.96	J/mol×K	1129.58	Joback Method
cpg	1556.03	J/mol×K	1167.11	Joback Method
cpg	1595.24	J/mol×K	1204.63	Joback Method

Sources

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=C30365652&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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