Dehydroergosterol

Inchi: InChI=1S/C28H42O/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: QSVJYFLQYMVBDR-JTVTWGPISA-N
Formula: C28H42O
SMILES: CC(C)C(C)C=CC(C)C1CCC2C3=CC=C4CC(O)CCC4(C)C3=CCC21C
Mol. weight [g/mol]: 394.63
CAS: 516-85-8

Physical Properties

Property code	Value	Unit	Source
gf	345.76	kJ/mol	Joback Method
hf	-262.63	kJ/mol	Joback Method
hfus	35.01	kJ/mol	Joback Method
hvap	94.16	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	7.251		Crippen Method
mcvol	350.610	ml/mol	McGowan Method
pc	1131.38	kPa	Joback Method
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook
rinpol	3214.90		NIST Webbook
rinpol	3214.90		NIST Webbook
tb	991.60	K	Joback Method
tc	1222.71	K	Joback Method
tf	553.62	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1292.94	J/mol×K	991.60	Joback Method
cpg	1324.47	J/mol×K	1030.12	Joback Method
cpg	1357.35	J/mol×K	1068.64	Joback Method
cpg	1391.97	J/mol×K	1107.16	Joback Method
cpg	1428.70	J/mol×K	1145.67	Joback Method

cpg	1467.94	J/mol×K	1184.19	Joback Method
cpg	1510.07	J/mol×K	1222.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C516858&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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