Ergosta-5,8,22-trien-3-ol, (3«beta»,22E)-

Other names: «delta»5,8(9),22-Ergostatrien-3«beta»-ol
Ergosta-5,8,22-trien-3«beta»-ol
Lichesterol
Ergostatrien-3«beta»-ol
5,8,22-Ergostatrienol
Ergosta-5,8(9),22-trien-3«beta»-ol

Inchi: InChI=1S/C28H44O/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: VILFZDAFELACSG-XLQBSWHXSA-N

Formula: C28H44O

SMILES: CC(C)C(C)C=CC(C)C1CCC2C3=C(CCC21C)C1(C)CCC(O)CC1=CC3

Mol. weight [g/mol]: 396.65

CAS: 50657-31-3

Physical Properties

Property code	Value	Unit	Source
gf	315.80	kJ/mol	Joback Method
hf	-320.41	kJ/mol	Joback Method
hfus	33.79	kJ/mol	Joback Method
hvap	93.87	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.475		Crippen Method
mcvol	354.910	ml/mol	McGowan Method
pc	1104.47	kPa	Joback Method
rinpol	3113.00		NIST Webbook
rinpol	3113.00		NIST Webbook
rinpol	3158.00		NIST Webbook
rinpol	3147.00		NIST Webbook
rinpol	3158.00		NIST Webbook
tb	992.44	K	Joback Method
tc	1222.94	K	Joback Method
tf	552.86	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1324.78	J/mol×K	992.44	Joback Method
cpg	1356.92	J/mol×K	1030.86	Joback Method
cpg	1390.33	J/mol×K	1069.27	Joback Method
cpg	1425.39	J/mol×K	1107.69	Joback Method
cpg	1462.49	J/mol×K	1146.11	Joback Method
cpg	1502.01	J/mol×K	1184.52	Joback Method
cpg	1544.33	J/mol×K	1222.94	Joback Method

Sources

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=C50657313&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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