

Ergost-8-en-3-ol, 14-methyl-, (3«beta»,5«alpha»)-

Other names:

5«alpha»-Ergost-8-en-3«beta»-ol, 14-methyl-
14«alpha»-Methyl-«delta»8-ergostenol
14-Methylergost-8-en-3-ol, (3«beta»,5«alpha»)-
14«alpha»-Methyl-5«alpha»-ergosten-8-3«beta»-ol

Inchi: InChI=1S/C29H50O/c1-19(2)20(3)8-9-21(4)24-13-16-29(7)26-11-10-22-18-23(30)12-15-2

InchiKey: PZDUAWZXRQLIQU-HXTUKQKFSA-N

Formula: C29H50O

SMILES: CC(C)C(C)CCC(C)C1CCC2(C)C3=C(CCC12C)C1(C)CCC(O)CC1CC3

Mol. weight [g/mol]: 414.71

CAS: 33860-48-9

Physical Properties

Property code	Value	Unit	Source
gf	210.47	kJ/mol	Joback Method
hf	-509.68	kJ/mol	Joback Method
hfus	30.12	kJ/mol	Joback Method
hvap	93.72	kJ/mol	Joback Method
log10ws	-8.84		Crippen Method
logp	8.169		Crippen Method
mcvol	377.600	ml/mol	McGowan Method
pc	997.65	kPa	Joback Method
tb	1002.59	K	Joback Method
tc	1232.00	K	Joback Method
tf	575.59	K	Joback Method
vc	1.427	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1464.10	J/molxK	1002.59	Joback Method
cpg	1503.14	J/molxK	1040.82	Joback Method
cpg	1544.31	J/molxK	1079.06	Joback Method
cpg	1588.09	J/molxK	1117.29	Joback Method
cpg	1634.94	J/molxK	1155.53	Joback Method

cpg	1685.32	J/mol×K	1193.76	Joback Method
cpg	1739.69	J/mol×K	1232.00	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=C33860489&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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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