Ergosta-5,22-dien-3-ol, acetate, (3.beta.,22e)-

Other names: Brassicasterol acetate
Inchi: InChI=1S/C30H48O2/c1-19(2)20(3)8-9-21(4)26-12-13-27-25-11-10-23-18-24(32-22(5)31)
InchiKey: YAXRKAKOIWXVHL-CMDGGOBGSA-N
Formula: C30H48O2
SMILES: CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)/C=C/C(C)C(C)C)CCC32)C1
Mol. weight [g/mol]: 440.71

Physical Properties

Property code	Value	Unit	Source
hfus	39.37	kJ/mol	Joback Method
hvap	135.98	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.38		Cheméo Relay (1.0)
logp	7.982		Crippen Method
mcvol	388.960	ml/mol	McGowan Method
rinpol	3224.00		NIST Webbook
tb	677.42	K	Cheméo Relay (1.0)
tf	435.10	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1477.08	J/mol×K	1003.85	Joback Method
cpg	1511.34	J/mol×K	1043.08	Joback Method
cpg	1546.51	J/mol×K	1082.31	Joback Method
cpg	1582.99	J/mol×K	1121.54	Joback Method
cpg	1621.14	J/mol×K	1160.76	Joback Method
cpg	1661.37	J/mol×K	1199.99	Joback Method
cpg	1704.06	J/mol×K	1239.22	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2458539&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point