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

Other names:	Ergosta-5,22-dien-3«beta»-ol
	Brassicasterin
	Brassicasterol
	«DELTA»5,22-Ergostadien-3«beta»-ol
	«DELTA»5,22-Ergostadienol
	ergosta-5,22(E)-dien-3«beta»-ol
Inchi:	InChI=1S/C28H46O/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:	OILXMJHPFNGGTO-JFPKDKPSSA-N
Formula:	C28H46O
SMILES:	CC(C)C(C)C=CC(C)C1CCC2C3CC=C4CC(O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	398.66
CAS:	474-67-9

Physical Properties

Property code	Value	Unit	Source
gf	289.68	kJ/mol	Joback Method
hf	-395.93	kJ/mol	Joback Method
hfus	35.49	kJ/mol	Joback Method
hvap	91.63	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	7.411		Crippen Method
mcvol	359.210	ml/mol	McGowan Method
pc	1053.46	kPa	Joback Method
rinpol	3063.00		NIST Webbook
rinpol	3078.00		NIST Webbook
rinpol	3055.00		NIST Webbook
rinpol	3088.00		NIST Webbook
rinpol	3080.00		NIST Webbook
rinpol	3038.00		NIST Webbook
rinpol	3085.00		NIST Webbook
rinpol	3088.00		NIST Webbook
rinpol	3044.00		NIST Webbook
rinpol	3115.00		NIST Webbook
rinpol	3115.00		NIST Webbook
rinpol	3047.00		NIST Webbook
rinpol	3088.00		NIST Webbook
rinpol	3085.00		NIST Webbook

rinpol	3063.00		NIST Webbook
tb	973.98	K	Joback Method
tc	1201.12	K	Joback Method
tf	518.58	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1359.87	J/mol×K	973.98	Joback Method
cpg	1391.77	J/mol×K	1011.84	Joback Method
cpg	1424.52	J/mol×K	1049.69	Joback Method
cpg	1458.49	J/mol×K	1087.55	Joback Method
cpg	1494.04	J/mol×K	1125.41	Joback Method
cpg	1531.52	J/mol×K	1163.26	Joback Method
cpg	1571.31	J/mol×K	1201.12	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=C474679&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