

Ergosta-4,22-dien-3-one

Other names:	Brassicasterone
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:	OWYXOXZSAKVGHJ-BQYQJAHWSA-N
Formula:	C28H44O
SMILES:	CC(C)C(C)C=CC(C)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	396.65
CAS:	4030-92-6

Physical Properties

Property code	Value	Unit	Source
gf	311.62	kJ/mol	Joback Method
hf	-361.06	kJ/mol	Joback Method
hfus	29.84	kJ/mol	Joback Method
hvap	79.51	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	7.619		Crippen Method
mcvol	354.910	ml/mol	McGowan Method
pc	1037.23	kPa	Joback Method
rinpol	3235.00		NIST Webbook
tb	954.29	K	Joback Method
tc	1194.90	K	Joback Method
tf	530.22	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1318.15	J/molxK	954.29	Joback Method
cpg	1350.90	J/molxK	994.39	Joback Method
cpg	1384.22	J/molxK	1034.49	Joback Method
cpg	1418.50	J/molxK	1074.60	Joback Method
cpg	1454.13	J/molxK	1114.70	Joback Method
cpg	1491.51	J/molxK	1154.80	Joback Method
cpg	1531.03	J/molxK	1194.90	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=C4030926&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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