5«alpha»-Stigmast-22-ene-3,6-dione

Inchi: InChI=1S/C29H46O2/c1-7-20(18(2)3)9-8-19(4)23-10-11-24-22-17-27(31)26-16-21(30)12
InchiKey: FJQGCLCMDPGZHC-GPRZXOKGSA-N
Formula: C29H46O2
SMILES: CCC(C=CC(C)C1CCC2C3CC(=O)C4CC(=O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	169.41	kJ/mol	Joback Method
hf	-586.05	kJ/mol	Joback Method
hfus	32.18	kJ/mol	Joback Method
hvap	84.72	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	7.268		Crippen Method
mcvol	374.870	ml/mol	McGowan Method
pc	964.47	kPa	Joback Method
rinpol	3598.00		NIST Webbook
rinpol	3598.00		NIST Webbook
tb	1036.18	K	Joback Method
tc	1283.61	K	Joback Method
tf	592.19	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1477.88	J/mol×K	1036.18	Joback Method
cpg	1513.24	J/mol×K	1077.42	Joback Method
cpg	1549.43	J/mol×K	1118.66	Joback Method
cpg	1586.83	J/mol×K	1159.89	Joback Method
cpg	1625.83	J/mol×K	1201.13	Joback Method
cpg	1666.81	J/mol×K	1242.37	Joback Method
cpg	1710.15	J/mol×K	1283.61	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=R641068&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