

5«alpha»-Stigmastan-3-one

Inchi: InChI=1S/C29H50O/c1-7-21(19(2)3)9-8-20(4)25-12-13-26-24-11-10-22-18-23(30)14-16-2
InchiKey: BVVFRHKBULZQCQ-YQDNUHGOSA-N
Formula: C29H50O
SMILES: CCC(CCC(C)C1CCC2C3CCC4CC(=O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 414.71

Physical Properties

Property code	Value	Unit	Source
gf	211.78	kJ/mol	Joback Method
hf	-565.57	kJ/mol	Joback Method
hfus	32.46	kJ/mol	Joback Method
hvap	80.51	kJ/mol	Joback Method
log10ws	-8.40		Crippen Method
logp	8.313		Crippen Method
mvol	377.600	ml/mol	McGowan Method
pc	914.39	kPa	Joback Method
rinpol	3370.00		NIST Webbook
rinpol	3370.00		NIST Webbook
tb	964.20	K	Joback Method
tc	1196.35	K	Joback Method
tf	529.05	K	Joback Method
vc	1.429	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1447.61	J/mol×K	964.20	Joback Method
cpg	1481.21	J/mol×K	1002.89	Joback Method
cpg	1515.03	J/mol×K	1041.58	Joback Method
cpg	1549.43	J/mol×K	1080.28	Joback Method
cpg	1584.73	J/mol×K	1118.97	Joback Method
cpg	1621.28	J/mol×K	1157.66	Joback Method
cpg	1659.43	J/mol×K	1196.35	Joback Method

Sources

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=R641122&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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