5«alpha»-Stigmast-22-en-3«beta»-ol

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: CSVWWLUMXNHWSU-LMDYIVHNSA-N
Formula: C29H50O
SMILES: CCC(C=CC(C)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 414.71

Physical Properties

Property code	Value	Unit	Source
gf	270.06	kJ/mol	Joback Method
hf	-483.22	kJ/mol	Joback Method
hfus	38.31	kJ/mol	Joback Method
hvap	92.59	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	7.881		Crippen Method
mcvol	377.600	ml/mol	McGowan Method
pc	957.91	kPa	Joback Method
rinpol	3253.00		NIST Webbook
tb	988.05	K	Joback Method
tc	1214.71	K	Joback Method
tf	512.33	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1463.75	J/mol×K	988.05	Joback Method
cpg	1497.33	J/mol×K	1025.83	Joback Method
cpg	1531.69	J/mol×K	1063.60	Joback Method
cpg	1567.22	J/mol×K	1101.38	Joback Method
cpg	1604.26	J/mol×K	1139.15	Joback Method
cpg	1643.19	J/mol×K	1176.93	Joback Method
cpg	1684.35	J/mol×K	1214.71	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=R641053&Units=SI
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
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

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