C29 5A,14B,17B,20S-Sterane

Inchi: InChI=1S/C29H52/c1-7-22(20(2)3)12-11-21(4)25-15-16-26-24-14-13-23-10-8-9-18-28(23
InchiKey: GKBHKNPLNHLYHT-DNUMLZFPSA-N
Formula: C29H52
SMILES: CCC(CCC(C)C1CCC2C3CCC4CCCCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 400.72

Physical Properties

Property code	Value	Unit	Source
gf	334.37	kJ/mol	Joback Method
hf	-427.87	kJ/mol	Joback Method
hfus	32.95	kJ/mol	Joback Method
hvap	76.27	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	9.134		Crippen Method
mcvol	376.030	ml/mol	McGowan Method
pc	895.34	kPa	Joback Method
rinpol	3001.00		NIST Webbook
tb	896.38	K	Joback Method
tc	1117.99	K	Joback Method
tf	460.83	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1388.02	J/mol×K	896.38	Joback Method
cpg	1420.71	J/mol×K	933.32	Joback Method
cpg	1453.24	J/mol×K	970.25	Joback Method
cpg	1485.96	J/mol×K	1007.19	Joback Method
cpg	1519.18	J/mol×K	1044.12	Joback Method
cpg	1553.25	J/mol×K	1081.06	Joback Method
cpg	1588.48	J/mol×K	1117.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56240&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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