

C27 5A,14A,17A,20S-Sterane

Inchi: InChI=1S/C27H48/c1-19(2)9-8-10-20(3)23-14-15-24-22-13-12-21-11-6-7-17-26(21,4)25(2,3)27
InchiKey: XIIAYQZJNBULGD-WENDITKYSA-N
Formula: C27H48
SMILES: CC(C)CCCC(C)C1CCC2C3CCC4CCCCC4(C)C3CCC12C
Mol. weight [g/mol]: 372.67

Physical Properties

Property code	Value	Unit	Source
gf	319.97	kJ/mol	Joback Method
hf	-381.31	kJ/mol	Joback Method
hfus	31.30	kJ/mol	Joback Method
hvap	72.20	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	8.498		Crippen Method
mcvol	347.850	ml/mol	McGowan Method
pc	1002.71	kPa	Joback Method
rinsol	2797.00		NIST Webbook
tb	851.06	K	Joback Method
tc	1072.72	K	Joback Method
tf	453.29	K	Joback Method
vc	1.317	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.75	J/molxK	851.06	Joback Method
cpg	1282.08	J/molxK	888.00	Joback Method
cpg	1312.99	J/molxK	924.95	Joback Method
cpg	1343.81	J/molxK	961.89	Joback Method
cpg	1374.86	J/molxK	998.83	Joback Method
cpg	1406.45	J/molxK	1035.78	Joback Method
cpg	1438.92	J/molxK	1072.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56129&Units=SI
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

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
mccvol:	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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