C28 5A,14A,17A,20S-Sterane

Inchi: InChI=1S/C28H50/c1-19(2)20(3)10-11-21(4)24-14-15-25-23-13-12-22-9-7-8-17-27(22,5)2
InchiKey: WAAWMJYYKITCGF-UXDOTZCHSA-N
Formula: C28H50
SMILES: CC(C)C(C)CCC(C)C1CCC2C3CCC4CCCCC4(C)C3CCC12C
Mol. weight [g/mol]: 386.70

Physical Properties

Property code	Value	Unit	Source
gf	325.95	kJ/mol	Joback Method
hf	-407.23	kJ/mol	Joback Method
hfus	30.36	kJ/mol	Joback Method
hvap	74.04	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.744		Crippen Method
mcvol	361.940	ml/mol	McGowan Method
pc	949.08	kPa	Joback Method
rinpol	2896.00		NIST Webbook
rinpol	2896.00		NIST Webbook
tb	873.50	K	Joback Method
tc	1096.28	K	Joback Method
tf	449.56	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.06	J/mol×K	873.50	Joback Method
cpg	1351.20	J/mol×K	910.63	Joback Method
cpg	1383.04	J/mol×K	947.76	Joback Method
cpg	1414.91	J/mol×K	984.89	Joback Method
cpg	1447.16	J/mol×K	1022.02	Joback Method
cpg	1480.10	J/mol×K	1059.15	Joback Method
cpg	1514.07	J/mol×K	1096.28	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56165&Units=SI

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