4-«alpha»-Methyl-5-«alpha»-cholestane

Other names: 4«alpha»-methylcholestane
Inchi: InChI=1S/C28H50/c1-19(2)9-7-10-20(3)24-14-15-25-22-12-13-23-21(4)11-8-17-27(23,5)2
InchiKey: AJHKOHJONNVXCK-ZDUMRXQFSA-N
Formula: C28H50
SMILES: CC(C)CCCC(C)C1CCC2C3CCC4C(C)CCCC4(C)C3CCC12C
Mol. weight [g/mol]: 386.70

Physical Properties

Property code	Value	Unit	Source
gf	320.68	kJ/mol	Joback Method
hf	-422.29	kJ/mol	Joback Method
hfus	34.96	kJ/mol	Joback Method
hvap	74.12	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.744		Crippen Method
mcvol	361.940	ml/mol	McGowan Method
pc	925.55	kPa	Joback Method
rinpol	2912.00		NIST Webbook
rinpol	2912.00		NIST Webbook
tb	869.27	K	Joback Method
tc	1089.19	K	Joback Method
tf	460.32	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.91	J/mol×K	869.27	Joback Method
cpg	1352.91	J/mol×K	905.92	Joback Method
cpg	1384.54	J/mol×K	942.58	Joback Method
cpg	1416.11	J/mol×K	979.23	Joback Method
cpg	1447.93	J/mol×K	1015.88	Joback Method
cpg	1480.30	J/mol×K	1052.53	Joback Method
cpg	1513.54	J/mol×K	1089.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R215055&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

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