4,14-dimethylcholestane

Inchi: InChI=1S/C29H52/c1-20(2)10-8-11-22(4)24-15-18-29(7)26-14-13-23-21(3)12-9-17-27(23
InchiKey: XZFBGOMDJSAVQA-BWBBPVGKSA-N
Formula: C29H52
SMILES: CC(C)CCCC(C)C1CCC2(C)C3CCC4C(C)CCCC4(C)C3CCC12C
Mol. weight [g/mol]: 400.72

Physical Properties

Property code	Value	Unit	Source
gf	323.61	kJ/mol	Joback Method
hf	-427.69	kJ/mol	Joback Method
hfus	31.25	kJ/mol	Joback Method
hvap	75.20	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	9.134		Crippen Method
mcvol	376.030	ml/mol	McGowan Method
pc	897.49	kPa	Joback Method
rinpol	3046.00		NIST Webbook
tb	892.39	K	Joback Method
tc	1115.87	K	Joback Method
tf	495.49	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1388.31	J/mol×K	892.39	Joback Method
cpg	1423.88	J/mol×K	929.64	Joback Method
cpg	1460.03	J/mol×K	966.88	Joback Method
cpg	1497.20	J/mol×K	1004.13	Joback Method
cpg	1535.80	J/mol×K	1041.38	Joback Method
cpg	1576.26	J/mol×K	1078.63	Joback Method
cpg	1619.00	J/mol×K	1115.87	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=R406023&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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