5-«alpha»-Cholest-8-3-«beta»-ol

Inchi: InChI=1S/C27H46O/c1-18(2)7-6-8-19(3)23-11-12-24-22-10-9-20-17-21(28)13-15-26(20,4
InchiKey: QETLKNDKQOXZRP-TVBVRADDSA-N
Formula: C27H46O
SMILES: CC(C)CCCC(C)C1CCC2C3=C(CCC21C)C1(C)CCC(O)CC1CC3
Mol. weight [g/mol]: 386.65

Physical Properties

Property code	Value	Unit	Source
gf	201.56	kJ/mol	Joback Method
hf	-478.36	kJ/mol	Joback Method
hfus	34.76	kJ/mol	Joback Method
hvap	90.81	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	7.533		Crippen Method
mcvol	349.420	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	3145.00		NIST Webbook
tb	957.03	K	Joback Method
tc	1179.28	K	Joback Method
tf	544.15	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.11	J/mol×K	957.03	Joback Method
cpg	1345.55	J/mol×K	994.07	Joback Method
cpg	1376.61	J/mol×K	1031.11	Joback Method
cpg	1408.61	J/mol×K	1068.16	Joback Method
cpg	1441.88	J/mol×K	1105.20	Joback Method
cpg	1476.73	J/mol×K	1142.24	Joback Method
cpg	1513.49	J/mol×K	1179.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R490543&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