Cholest-1-en-3-one, (5«alpha»)-

Other names: 5«alpha»-Cholest-1-en-3-one
17-(1,5-Dimethylhexyl)-10,13-dimethyl-4,5,6,7,8,9,10,11,12,13,14,15,16,17-tetradecahyd
5-alpha-Cholest-1-en-3-one
Inchi: InChI=1S/C27H44O/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: IIPHPVVRBVBREZ-WZQCNCHSSA-N
Formula: C27H44O
SMILES: CC(C)CCCC(C)C1CCC2C3CCC4CC(=O)C=CC4(C)C3CCC12C
Mol. weight [g/mol]: 384.64
CAS: 601-55-8

Physical Properties

Property code	Value	Unit	Source
gf	227.34	kJ/mol	Joback Method
hf	-461.23	kJ/mol	Joback Method
hfus	32.03	kJ/mol	Joback Method
hvap	76.74	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	7.453		Crippen Method
mcvol	345.120	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
tb	918.04	K	Joback Method
tc	1150.89	K	Joback Method
tf	522.27	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.71	J/mol×K	918.04	Joback Method
cpg	1308.92	J/mol×K	956.85	Joback Method
cpg	1340.16	J/mol×K	995.66	Joback Method
cpg	1371.77	J/mol×K	1034.46	Joback Method
cpg	1404.10	J/mol×K	1073.27	Joback Method
cpg	1437.46	J/mol×K	1112.08	Joback Method

cpg	1472.21	J/mol×K	1150.89	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=C601558&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume