Cholic acid

Other names:	17«beta»-(1-Methyl-3-carboxypropyl)etiocholane-3«alpha»,7«alpha»,12«alpha»-triol 17Â«betaÂ»-(1-Methyl-3-carboxypropyl)etiocholane-3Â«alphaÂ»,7Â«alphaÂ»,12Â«alpha 3,7,12-Trihydroxy-cholan-24-oic acid, (3«alpha»,5«beta»,7«alpha»,12«alpha»)- 3,7,12-Trihydroxy-cholan-24-oic acid, (3Â«alphaÂ»,5Â«betaÂ»,7Â«alphaÂ»,12Â«alphaÂ»)- 3-«alpha»,7-«alpha»,12-«alpha»-Trihydroxy-5-«beta»-cholan-24-oic acid 3-«alpha»,7-«alpha»,12-«alpha»-Trihydroxycholansaeure 3-Â«alphaÂ»,7-Â«alphaÂ»,12-Â«alphaÂ»-Trihydroxy-5-Â«betaÂ»-cholan-24-oic acid 3-Â«alphaÂ»,7-Â«alphaÂ»,12-Â«alphaÂ»-Trihydroxycholansaeure 3«alpha»,7«alpha»,12«alpha»-Trihydroxy-5«beta»-Cholanic acid 3Â«alphaÂ»,7Â«alphaÂ»,12Â«alphaÂ»-Trihydroxy-5Â«betaÂ»-Cholanic acid 5«beta»-Cholan-24-oic acid, 3«alpha»,7«alpha»,12«alpha»-trihydroxy- 5«beta»-Cholic acid 5Â«betaÂ»-Cholan-24-oic acid, 3Â«alphaÂ»,7Â«alphaÂ»,12Â«alphaÂ»-trihydroxy- 5Â«betaÂ»-Cholic acid Cholalic acid Cholalin Cholan-24-oic acid, 3,7,12-trihydroxy-, (3«alpha»,5«beta»,7«alpha»,12«alpha»)- Cholan-24-oic acid, 3,7,12-trihydroxy-, (3Â«alphaÂ»,5Â«betaÂ»,7Â«alphaÂ»,12Â«alphaÂ»)- Cholsaeure Colalin NSC-6135
Inchi:	InChI=1S/C25H42O5/c1-14(5-8-21(29)30)16-6-7-17-22-18(11-20(28)25(16,17)4)24(3)10-
InchiKey:	ZSNMWSXGJNFSAV-HAVJKBGOSA-N
Formula:	C24H40O5
SMILES:	CC(CCC(=O)O)C1CCC2C3C(O)CC4(C)CC(O)CCC4(C)C3CC(O)C12C
Mol. weight [g/mol]:	408.57
CAS:	81-25-4

Physical Properties

Property code	Value	Unit	Source
gf	-399.25	kJ/mol	Joback Method
hf	-1102.03	kJ/mol	Joback Method
hfus	44.51	kJ/mol	Joback Method
hvap	139.52	kJ/mol	Joback Method
log10ws	-3.37		Aqueous Solubility Prediction Method
logp	3.839		Crippen Method

mcvol	344.720	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
tb	1214.56	K	Joback Method
tc	1518.63	K	Joback Method
tf	439.00 ± 4.00	K	NIST Webbook
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1596.14	J/mol×K	1214.56	Joback Method
cpg	1666.32	J/mol×K	1265.24	Joback Method
cpg	1744.38	J/mol×K	1315.92	Joback Method
cpg	1831.33	J/mol×K	1366.59	Joback Method
cpg	1928.17	J/mol×K	1417.27	Joback Method
cpg	2035.91	J/mol×K	1467.95	Joback Method
cpg	2155.56	J/mol×K	1518.63	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C81254&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume