Dehydrocholic acid

Other names:

Cholan-24-oic acid, 3,7,12-trioxo-, (5«beta»)-
5«beta»-Cholan-24-oic acid, 3,7,12-trioxo-
Acolen
Bilidren
Bilostat
Cholagon
Cholic acid, dehydro-
Cholimed
Chologon
Decholin
Dehychol
Dehycol
Dehycon
Dehydrocholate
Dehystolin
Deidrocolico Vita
Didocol
Didrocolo
Dilabil
Drenobyl
DHC
Erebile
Felacrinos
Hykolex
Ketocholanic Acid
Novocolin
Oxycholin
Procholon
Sanocholen
Triketocholanic acid
3,7,12-Triketo-5«beta»-cholanic acid
3,7,12-Triketo-5«beta»-cholanoic acid
3,7,12-Triketocholanic acid
3,7,12-Trioxo-5«beta»-cholanic acid
3,7,12-Trioxocholanic acid
5«beta»-Cholanic acid, 3,7,12-trioxo-
Biochol
Cholan DH
Dee-Co
Doxycholpotassium

	Ketochol
	Khologon
	3,7,12-Trioxo-5«beta»-cholan-24-oic acid
	Acide dehydrocholique
	Dehydrocholsaeure
	Dilahil
	Atrocholin
	3,7,12-Trioxo-24-cholanic acid
	Cholepatin
	3,7,12-Tri-keto-5«beta»-Cholan-24-oic acid
	Hydrochol
Inchi:	InChI=1S/C24H34O5/c1-13(4-7-21(28)29)16-5-6-17-22-18(12-20(27)24(16,17)3)23(2)9-8
InchiKey:	OHXPGWPVLFPUSM-FLXXOENNSA-N
Formula:	C24H34O5
SMILES:	CC(CCC(=O)O)C1CCC2C3C(=O)CC4CC(=O)CCC4(C)C3CC(=O)C12C
Mol. weight [g/mol]:	402.52
CAS:	81-23-2

Physical Properties

Property code	Value	Unit	Source
gf	-336.36	kJ/mol	Joback Method
hf	-992.02	kJ/mol	Joback Method
hfus	31.27	kJ/mol	Joback Method
hvap	102.08	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.073		Crippen Method
mcvol	317.730	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
tb	1132.37	K	Joback Method
tc	1390.48	K	Joback Method
tf	749.89	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.72	J/mol×K	1132.37	Joback Method

cpg	1353.02	J/mol×K	1175.39	Joback Method
cpg	1386.58	J/mol×K	1218.41	Joback Method
cpg	1421.72	J/mol×K	1261.42	Joback Method
cpg	1458.77	J/mol×K	1304.44	Joback Method
cpg	1498.06	J/mol×K	1347.46	Joback Method
cpg	1539.93	J/mol×K	1390.48	Joback Method

Sources

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=C81232&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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