

Glycocholic acid

Other names:

Glycine,
N-[(3«alpha»,5«beta»,7«alpha»,12«alpha»)-3,7,12-trihydroxy-24-oxocholan-24-yl]-
Glycine,
N-[(3Â«alphaÂ»,5Â«betaÂ»,7Â«alphaÂ»,12Â«alphaÂ»)-3,7,12-trihydroxy-24-oxocholan-
N-(3-«alpha»,7-«alpha»,12-«alpha»-trihydroxycholan-24-oyl)glycine
N-(3-Â«alphaÂ»,7-Â«alphaÂ»,12-Â«alphaÂ»-trihydroxycholan-24-oyl)glycine

Inchi: InChI=1S/C26H43NO6/c1-14(4-7-22(31)27-13-23(32)33)17-5-6-18-24-19(12-21(30)26(1**InchiKey:** RFDAIACWWDREDC-FFFROSDMSA-N**Formula:** C26H43NO6**SMILES:** CC(CCC(O)=NCC(=O)O)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CC(O)C12C**Mol. weight [g/mol]:** 465.62**CAS:** 475-31-0

Physical Properties

Property code	Value	Unit	Source
hf	-1217.71	kJ/mol	Joback Method
hvap	162.97	kJ/mol	Joback Method
log10ws	-5.15		Aqueous Solubility Prediction Method
logp	3.405		Crippen Method
mcvol	370.360	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
tb	1405.94	K	Joback Method
tc	1869.64	K	Joback Method
tf	439.65	K	Aqueous Solubility Prediction Method

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C475310&Units=SI>**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

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