

Methyl-3beta,7beta,12beta-trihydroxy-5beta-chola

Inchi:	InChI=1S/C25H42O5/c1-14(5-8-22(29)30-4)17-6-7-18-23-19(13-21(28)25(17,18)3)24(2)1
InchiKey:	DLYVTEULDNMQAR-UHFFFAOYSA-N
Formula:	C25H42O5
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CC(O)C12C
Mol. weight [g/mol]:	422.60
CAS:	81702-93-4

Physical Properties

Property code	Value	Unit	Source
gf	-361.94	kJ/mol	Joback Method
hf	-1097.26	kJ/mol	Joback Method
hfus	47.90	kJ/mol	Joback Method
hvap	126.40	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.537		Crippen Method
mcvol	344.720	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
tb	1144.56	K	Joback Method
tc	1412.67	K	Joback Method
tf	687.65	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.41	J/molxK	1144.56	Joback Method
cpg	1514.54	J/molxK	1189.24	Joback Method
cpg	1557.15	J/molxK	1233.93	Joback Method
cpg	1602.74	J/molxK	1278.61	Joback Method
cpg	1651.80	J/molxK	1323.30	Joback Method
cpg	1704.82	J/molxK	1367.98	Joback Method
cpg	1762.30	J/molxK	1412.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81702934&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

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

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