3Beta,7beta,12beta-trihydroxy-5beta-cholan-24-oi acid

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-CSFDPCLMSA-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: 81873-90-7

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	-5.16		Crippen 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	750.14	K	Joback Method
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=C81873907&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
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