Methyl 5-«beta»-cholan-3-«alpha»,7-«alpha»-diol-12-one-

Inchi: InChI=1S/C25H40O5/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: LGWDBNNCYKGKFM-ZGPVKVJISA-N

Formula: C25H40O5

SMILES: COC(=O)CCC(C)C1CCC2C3C(O)CC4CC(O)CCC4(C)C3CC(=O)C12C

Mol. weight [g/mol]: 420.58

Physical Properties

Property code	Value	Unit	Source
gf	-340.00	kJ/mol	Joback Method
hf	-1062.39	kJ/mol	Joback Method
hfus	42.26	kJ/mol	Joback Method
hvap	114.28	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.745		Crippen Method
mcvol	340.420	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	3402.00		NIST Webbook
rinpol	3402.00		NIST Webbook
tb	1124.87	K	Joback Method
tc	1378.07	K	Joback Method
tf	699.29	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1427.29	J/mol×K	1124.87	Joback Method
cpg	1462.29	J/mol×K	1167.07	Joback Method
cpg	1498.88	J/mol×K	1209.27	Joback Method
cpg	1537.43	J/mol×K	1251.47	Joback Method
cpg	1578.33	J/mol×K	1293.67	Joback Method
cpg	1621.94	J/mol×K	1335.87	Joback Method
cpg	1668.65	J/mol×K	1378.07	Joback Method

Sources

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=R215897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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