

Methyl 5-«beta»-cholan-3-«alpha»-ol-12-one-24-oate

Inchi: InChI=1S/C25H40O4/c1-15(5-10-23(28)29-4)19-8-9-20-18-7-6-16-13-17(26)11-12-24(16)
InchiKey: BNXXKGNFJUFIND-OBBNEJRQSA-N
Formula: C25H40O4
SMILES: COC(=O)CCC(C)C1CCC2C3CCC4CC(O)CCC4(C)C3CC(=O)C12C
Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-195.47	kJ/mol	Joback Method
hf	-889.82	kJ/mol	Joback Method
hfus	37.10	kJ/mol	Joback Method
hvap	97.91	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.774		Crippen Method
mcvol	334.550	ml/mol	McGowan Method
pc	1245.09	kPa	Joback Method
rinpol	3308.00		NIST Webbook
rinpol	3308.00		NIST Webbook
tb	1037.36	K	Joback Method
tc	1274.40	K	Joback Method
tf	642.71	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.80	J/mol×K	1037.36	Joback Method
cpg	1363.62	J/mol×K	1076.87	Joback Method
cpg	1395.25	J/mol×K	1116.37	Joback Method
cpg	1427.99	J/mol×K	1155.88	Joback Method
cpg	1462.15	J/mol×K	1195.39	Joback Method
cpg	1498.07	J/mol×K	1234.90	Joback Method
cpg	1536.04	J/mol×K	1274.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R215911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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