

Cholan-24-oic acid, 3,7,12-trioxo-, methyl ester

Other names:	Methyl cholan-3,7,12-trione-24-oate Methyl 5-«beta»-cholan-3,7,12-trione-24-oate
Inchi:	InChI=1S/C25H36O5/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:	ZNRVRJLOYAQJBW-RBWRVWNOSA-N
Formula:	C25H36O5
SMILES:	COC(=O)CCC(C)C1CCC2C3C(=O)CC4CC(=O)CCC4(C)C3CC(=O)C12C
Mol. weight [g/mol]:	416.55
CAS:	55555-42-5

Physical Properties

Property code	Value	Unit	Source
gf	-296.12	kJ/mol	Joback Method
hf	-992.65	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	90.04	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.162		Crippen Method
mcvol	331.820	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpol	3392.00		NIST Webbook
rinpol	3392.00		NIST Webbook
tb	1085.49	K	Joback Method
tc	1343.01	K	Joback Method
tf	722.57	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1338.58	J/mol×K	1085.49	Joback Method
cpg	1369.69	J/mol×K	1128.41	Joback Method
cpg	1401.35	J/mol×K	1171.33	Joback Method
cpg	1433.85	J/mol×K	1214.25	Joback Method
cpg	1467.51	J/mol×K	1257.17	Joback Method

cpg	1502.63	J/mol×K	1300.09	Joback Method
cpg	1539.52	J/mol×K	1343.01	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55555425&Units=SI

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
hvac:	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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