Methyl 5-«beta»-cholan-3,7-dione-24-oate

Inchi: InChI=1S/C25H38O4/c1-15(5-8-22(28)29-4)18-6-7-19-23-20(10-12-25(18,19)3)24(2)11-9
InchiKey: UZRRNRRCPZZPNY-WHOPQXHASA-N
Formula: C25H38O4
SMILES: COC(=O)CCC(C)C1CCC2C3C(=O)CC4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-173.53	kJ/mol	Joback Method
hf	-854.95	kJ/mol	Joback Method
hfus	31.45	kJ/mol	Joback Method
hvap	85.79	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.983		Crippen Method
mcvol	330.250	ml/mol	McGowan Method
pc	1224.27	kPa	Joback Method
rinpol	3269.00		NIST Webbook
tb	1017.67	K	Joback Method
tc	1264.96	K	Joback Method
tf	654.35	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.03	J/mol×K	1017.67	Joback Method
cpg	1321.80	J/mol×K	1058.89	Joback Method
cpg	1353.00	J/mol×K	1100.10	Joback Method
cpg	1384.95	J/mol×K	1141.32	Joback Method
cpg	1417.98	J/mol×K	1182.53	Joback Method
cpg	1452.40	J/mol×K	1223.75	Joback Method
cpg	1488.53	J/mol×K	1264.96	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=R490563&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
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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