Methyl chol-4,6-dien-3-one-24-oate

Inchi: InChI=1S/C25H36O3/c1-16(5-10-23(27)28-4)20-8-9-21-19-7-6-17-15-18(26)11-13-24(17
InchiKey: OSRBYFQAFFCYCV-UHFFFAOYSA-N
Formula: C25H36O3
SMILES: COC(=O)CCC(C)C1CCC2C3C=CC4=CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 384.55

Physical Properties

Property code	Value	Unit	Source
gf	7.06	kJ/mol	Joback Method
hf	-592.82	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	83.10	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.500		Crippen Method
mcvol	320.080	ml/mol	McGowan Method
pc	1272.78	kPa	Joback Method
rinpol	3253.00		NIST Webbook
tb	957.82	K	Joback Method
tc	1198.44	K	Joback Method
tf	604.41	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.05	J/mol×K	957.82	Joback Method
cpg	1204.96	J/mol×K	997.92	Joback Method
cpg	1234.39	J/mol×K	1038.03	Joback Method
cpg	1264.66	J/mol×K	1078.13	Joback Method
cpg	1296.11	J/mol×K	1118.23	Joback Method
cpg	1329.10	J/mol×K	1158.34	Joback Method
cpg	1363.95	J/mol×K	1198.44	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=R216058&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