«DELTA»6-Lithocholic acid, acetate-methyl ester

Inchi: InChI=1S/C27H42O4/c1-17(6-11-25(29)30-5)22-9-10-23-21-8-7-19-16-20(31-18(2)28)12
InchiKey: ZUXCJTMUJNGXDG-YOKQTMLGSA-N
Formula: C27H42O4
SMILES: COC(=O)CCC(C)C1CCC2C3C=CC4CC(OC(C)=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 430.62

Physical Properties

Property code	Value	Unit	Source
gf	-123.18	kJ/mol	Joback Method
hf	-828.19	kJ/mol	Joback Method
hfus	42.69	kJ/mol	Joback Method
hvap	90.89	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.942		Crippen Method
mcvol	358.430	ml/mol	McGowan Method
pc	1060.33	kPa	Joback Method
rinpol	3136.00		NIST Webbook
tb	998.57	K	Joback Method
tc	1232.23	K	Joback Method
tf	609.13	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1364.58	J/mol×K	998.57	Joback Method
cpg	1395.27	J/mol×K	1037.51	Joback Method
cpg	1426.53	J/mol×K	1076.46	Joback Method
cpg	1458.67	J/mol×K	1115.40	Joback Method
cpg	1492.03	J/mol×K	1154.35	Joback Method
cpg	1526.93	J/mol×K	1193.29	Joback Method
cpg	1563.69	J/mol×K	1232.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R182237&Units=SI
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

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