Isoursodeoxycholic acid, acetate-methyl ester

Inchi: InChI=1S/C29H46O6/c1-17(7-10-26(32)33-6)22-8-9-23-27-24(12-14-29(22,23)5)28(4)13-
InchiKey: ZKHVKSAMEUAGEN-HNVCCVSMSA-N
Formula: C29H46O6
SMILES: COC(=O)CCC(C)C1CCC2C3C(OC(C)=O)CC4CC(OC(C)=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 490.67

Physical Properties

Property code	Value	Unit	Source
gf	-377.93	kJ/mol	Joback Method
hf	-1192.39	kJ/mol	Joback Method
hfus	50.50	kJ/mol	Joback Method
hvap	103.89	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.708		Crippen Method
mcvol	398.350	ml/mol	McGowan Method
pc	926.11	kPa	Joback Method
rinpol	3405.00		NIST Webbook
tb	1116.79	K	Joback Method
tc	1367.31	K	Joback Method
tf	698.83	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1610.75	J/mol×K	1116.79	Joback Method
cpg	1646.27	J/mol×K	1158.54	Joback Method
cpg	1682.95	J/mol×K	1200.30	Joback Method
cpg	1721.15	J/mol×K	1242.05	Joback Method
cpg	1761.24	J/mol×K	1283.81	Joback Method
cpg	1803.59	J/mol×K	1325.56	Joback Method
cpg	1848.57	J/mol×K	1367.31	Joback Method

Sources

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=R182653&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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