

Isochenodeoxycholic 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-JCTYIVIQSA-N
Formula:	C29H46O6
SMILES:	<chem>COC(=O)CCC(C)C1CCC2C3C(OC(C)=O)CC4CC(OC(C)=O)CCC4(C)C3CCC12C</chem>
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
mvol	398.350	ml/mol	McGowan Method
pc	926.11	kPa	Joback Method
rinpol	3319.00		NIST Webbook
rinpol	3319.00		NIST Webbook
tb	1116.79	K	Joback Method
tc	1367.31	K	Joback Method
tf	698.83	K	Joback Method
vc	1.504	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R182613&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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