Homochenodeoxycholic acid, acetate-methyl ester

Inchi: InChI=1S/C30H48O6/c1-18(8-7-9-27(33)34-6)23-10-11-24-28-25(13-15-30(23,24)5)29(4
InchiKey: FZQNQAANPWUHFK-MMRPWILXSA-N
Formula: C30H48O6
SMILES: COC(=O)CCCC(C)C1CCC2C3C(OC(C)=O)CC4CC(OC(C)=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 504.70

Physical Properties

Property code	Value	Unit	Source
gf	-369.51	kJ/mol	Joback Method
hf	-1213.03	kJ/mol	Joback Method
hfus	53.09	kJ/mol	Joback Method
hvap	106.12	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.098		Crippen Method
mcvol	412.440	ml/mol	McGowan Method
pc	874.28	kPa	Joback Method
rinpol	3408.00		NIST Webbook
rinpol	3408.00		NIST Webbook
tb	1139.67	K	Joback Method
tc	1395.58	K	Joback Method
tf	710.10	K	Joback Method
vc	1.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1684.41	J/mol×K	1139.67	Joback Method
cpg	1722.03	J/mol×K	1182.32	Joback Method
cpg	1761.03	J/mol×K	1224.97	Joback Method
cpg	1801.80	J/mol×K	1267.63	Joback Method
cpg	1844.75	J/mol×K	1310.28	Joback Method
cpg	1890.27	J/mol×K	1352.93	Joback Method
cpg	1938.77	J/mol×K	1395.58	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=R182519&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