Norursodeoxycholic acid, acetate-methyl ester

Inchi: InChI=1S/C28H44O6/c1-16(13-25(31)32-6)21-7-8-22-26-23(10-12-28(21,22)5)27(4)11-9-
InchiKey: SSSUNRYYXMSDPC-LQYZRRBISA-N
Formula: C28H44O6
SMILES: COC(=O)CC(C)C1CCC2C3C(OC(C)=O)CC4CC(OC(C)=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 476.65

Physical Properties

Property code	Value	Unit	Source
gf	-386.35	kJ/mol	Joback Method
hf	-1171.75	kJ/mol	Joback Method
hfus	47.91	kJ/mol	Joback Method
hvap	101.67	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.318		Crippen Method
mcvol	384.260	ml/mol	McGowan Method
pc	982.69	kPa	Joback Method
rinpol	3281.00		NIST Webbook
tb	1093.91	K	Joback Method
tc	1340.23	K	Joback Method
tf	687.56	K	Joback Method
vc	1.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1538.14	J/mol×K	1093.91	Joback Method
cpg	1571.85	J/mol×K	1134.96	Joback Method
cpg	1606.53	J/mol×K	1176.02	Joback Method
cpg	1642.51	J/mol×K	1217.07	Joback Method
cpg	1680.14	J/mol×K	1258.12	Joback Method
cpg	1719.76	J/mol×K	1299.18	Joback Method
cpg	1761.73	J/mol×K	1340.23	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=R182777&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