Homocholic acid, acetate-methyl ester

Inchi: InChI=1S/C32H50O8/c1-18(9-8-10-29(36)37-7)24-11-12-25-30-26(17-28(32(24,25)6)40-
InchiKey: ZIGHEEYIWXXOSP-MXQUNYRJSA-N
Formula: C32H50O8
SMILES: COC(=O)CCCC(C)C1CCC2C3C(OC(C)=O)CC4CC(OC(C)=O)CCC4(C)C3CC(OC(C)=O
Mol. weight [g/mol]: 562.73

Physical Properties

Property code	Value	Unit	Source
gf	-594.30	kJ/mol	Joback Method
hf	-1519.45	kJ/mol	Joback Method
hfus	62.13	kJ/mol	Joback Method
hvap	119.42	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.640		Crippen Method
mcvol	448.060	ml/mol	McGowan Method
pc	788.60	kPa	Joback Method
rinpol	3435.00		NIST Webbook
rinpol	3435.00		NIST Webbook
tb	1257.05	K	Joback Method
tc	1552.55	K	Joback Method
tf	800.56	K	Joback Method
vc	1.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1904.41	J/mol×K	1257.05	Joback Method
cpg	1950.18	J/mol×K	1306.30	Joback Method
cpg	1998.40	J/mol×K	1355.55	Joback Method
cpg	2049.64	J/mol×K	1404.80	Joback Method
cpg	2104.47	J/mol×K	1454.05	Joback Method
cpg	2163.45	J/mol×K	1503.30	Joback Method
cpg	2227.14	J/mol×K	1552.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R182539&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