«alpha»-Muricholic acid, acetate-methyl ester

Inchi: InChI=1S/C31H48O8/c1-17(8-11-26(35)36-7)22-9-10-23-27-24(13-15-30(22,23)5)31(6)14
InchiKey: SCZJGLWPRVUGAT-NVVKZUAYSA-N
Formula: C31H48O8
SMILES: COC(=O)CCC(C)C1CCC2C3C(OC(C)=O)C(OC(C)=O)C4CC(OC(C)=O)CCC4(C)C3CC
Mol. weight [g/mol]: 548.71

Physical Properties

Property code	Value	Unit	Source
gf	-602.72	kJ/mol	Joback Method
hf	-1498.81	kJ/mol	Joback Method
hfus	59.54	kJ/mol	Joback Method
hvap	117.19	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.249		Crippen Method
mcvol	433.970	ml/mol	McGowan Method
pc	832.90	kPa	Joback Method
rinpol	3471.00		NIST Webbook
rinpol	3471.00		NIST Webbook
tb	1234.17	K	Joback Method
tc	1518.97	K	Joback Method
tf	789.29	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1827.98	J/mol×K	1234.17	Joback Method
cpg	1870.45	J/mol×K	1281.64	Joback Method
cpg	1914.97	J/mol×K	1329.10	Joback Method
cpg	1962.05	J/mol×K	1376.57	Joback Method
cpg	2012.18	J/mol×K	1424.04	Joback Method
cpg	2065.86	J/mol×K	1471.51	Joback Method
cpg	2123.59	J/mol×K	1518.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R182193&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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