3«alpha»,6«beta»,7«beta»,12«beta»-Tetrahydroxy
acid, acetate-methyl ester

Inchi: InChI=1S/C33H50O10/c1-17(9-12-28(38)39-8)23-10-11-24-29-25(16-27(33(23,24)7)41-1

InchiKey: NDZQWHMQQJDYRD-UAPZMJKZSA-N

Formula: C33H50O10

SMILES: COC(=O)CCC(C)C1CCC2C3C(OC(C)=O)C(OC(C)=O)C4CC(OC(C)=O)CCC4(C)C3CC(

Mol. weight [g/mol]: 606.74

Physical Properties

Property code	Value	Unit	Source
gf	-827.51	kJ/mol	Joback Method
hf	-1805.23	kJ/mol	Joback Method
hfus	68.58	kJ/mol	Joback Method
hvap	130.49	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	4.791		Crippen Method
mcvol	469.590	ml/mol	McGowan Method
pc	753.08	kPa	Joback Method
rinpol	3696.00		NIST Webbook
tb	1351.55	K	Joback Method
tc	1693.42	K	Joback Method
tf	879.75	K	Joback Method
vc	1.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2042.51	J/mol×K	1351.55	Joback Method
cpg	2094.96	J/mol×K	1408.53	Joback Method
cpg	2150.91	J/mol×K	1465.51	Joback Method
cpg	2211.16	J/mol×K	1522.48	Joback Method
cpg	2276.49	J/mol×K	1579.46	Joback Method
cpg	2347.67	J/mol×K	1636.44	Joback Method
cpg	2425.51	J/mol×K	1693.42	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=R182371&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