GA3-13-O-glucoside, permethylated

Inchi: InChI=1S/C31H44O11/c1-16-13-29-15-30(16,41-26-23(38-7)22(37-6)21(36-5)17(40-26)1
InchiKey: LNVOHHIQKUEONS-VWAQXLAKSA-N
Formula: C31H44O11
SMILES: C=C1CC23CC1(OC1OC(COC)C(OC)C(OC)C1OC)CCC2C12C=CC(OC)C(C)(C(=O)O1)C
Mol. weight [g/mol]: 592.67

Physical Properties

Property code	Value	Unit	Source
gf	-637.50	kJ/mol	Joback Method
hf	-1656.39	kJ/mol	Joback Method
hfus	62.11	kJ/mol	Joback Method
hvap	115.50	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.210		Crippen Method
mcvol	429.860	ml/mol	McGowan Method
pc	905.06	kPa	Joback Method
rinpol	3515.00		NIST Webbook
tb	1269.59	K	Joback Method
tc	1558.60	K	Joback Method
tf	936.43	K	Joback Method
vc	1.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2021.95	J/mol×K	1269.59	Joback Method
cpg	2101.70	J/mol×K	1317.76	Joback Method
cpg	2188.98	J/mol×K	1365.93	Joback Method
cpg	2284.63	J/mol×K	1414.10	Joback Method
cpg	2389.48	J/mol×K	1462.27	Joback Method
cpg	2504.38	J/mol×K	1510.43	Joback Method
cpg	2630.16	J/mol×K	1558.60	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=R297502&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