3-epi-GA1-3«alpha»-O-glucoside, permethylated

Inchi: InChI=1S/C31H46O11/c1-16-13-29-15-30(16,39-8)11-9-18(29)31-12-10-19(28(2,27(33)4

InchiKey: IMGCILBAQGOKMI-YKCBFNPQSA-N

Formula: C31H46O11

SMILES: C=C1CC23CC1(OC)CCC2C12CCC(OC4OC(COC)C(OC)C(OC)C4OC)C(C)(C(=O)O1)C

Mol. weight [g/mol]: 594.69

Physical Properties

Property code	Value	Unit	Source
gf	-667.46	kJ/mol	Joback Method
hf	-1714.17	kJ/mol	Joback Method
hfus	60.88	kJ/mol	Joback Method
hvap	115.21	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.434		Crippen Method
mcvol	434.160	ml/mol	McGowan Method
pc	885.77	kPa	Joback Method
rinpol	3625.00		NIST Webbook
rinpol	3625.00		NIST Webbook
tb	1270.43	K	Joback Method
tc	1560.31	K	Joback Method
tf	935.67	K	Joback Method
vc	1.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2057.50	J/mol×K	1270.43	Joback Method
cpg	2137.72	J/mol×K	1318.74	Joback Method
cpg	2225.40	J/mol×K	1367.06	Joback Method
cpg	2321.37	J/mol×K	1415.37	Joback Method
cpg	2426.48	J/mol×K	1463.68	Joback Method
cpg	2541.58	J/mol×K	1512.00	Joback Method
cpg	2667.51	J/mol×K	1560.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R297453&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

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