GA20-13-O-glucoside, permethylated

Inchi: InChI=1S/C30H44O10/c1-16-13-28-15-29(16,39-25-22(36-6)21(35-5)20(34-4)17(38-25)1
InchiKey: QEXOYMVZQLUEJN-IYHAUVRDSA-N
Formula: C30H44O10
SMILES: C=C1CC23CC1(OC1OC(COC)C(OC)C(OC)C1OC)CCC2C12CCCC(C)(C(=O)O1)C2C3C
Mol. weight [g/mol]: 564.66

Physical Properties

Property code	Value	Unit	Source
gf	-563.17	kJ/mol	Joback Method
hf	-1540.97	kJ/mol	Joback Method
hfus	56.04	kJ/mol	Joback Method
hvap	110.89	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	2.809		Crippen Method
mcvol	414.200	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	3398.00		NIST Webbook
rinpol	3398.00		NIST Webbook
tb	1229.80	K	Joback Method
tc	1506.20	K	Joback Method
tf	906.41	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1920.97	J/mol×K	1229.80	Joback Method
cpg	1994.22	J/mol×K	1275.87	Joback Method
cpg	2074.24	J/mol×K	1321.93	Joback Method
cpg	2161.81	J/mol×K	1368.00	Joback Method
cpg	2257.70	J/mol×K	1414.07	Joback Method
cpg	2362.69	J/mol×K	1460.14	Joback Method
cpg	2477.54	J/mol×K	1506.20	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=R297488&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