GA4-3«beta»-O-glucoside, permethylated

Inchi: InChI=1S/C30H44O10/c1-15-12-29-13-16(15)8-9-18(29)30-11-10-19(28(2,27(32)40-30)2
InchiKey: SLPPINDFMDFPTC-ACYHDOQYSA-N
Formula: C30H44O10
SMILES: C=C1CC23CC1CCC2C12CCC(OC4OC(COC)C(OC)C(OC)C4OC)C(C)(C(=O)O1)C2C3C
Mol. weight [g/mol]: 564.66

Physical Properties

Property code	Value	Unit	Source
gf	-565.39	kJ/mol	Joback Method
hf	-1576.55	kJ/mol	Joback Method
hfus	63.41	kJ/mol	Joback Method
hvap	111.73	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	2.665		Crippen Method
mcvol	414.200	ml/mol	McGowan Method
pc	922.74	kPa	Joback Method
rinpol	3440.00		NIST Webbook
rinpol	3440.00		NIST Webbook
tb	1224.89	K	Joback Method
tc	1501.05	K	Joback Method
tf	878.27	K	Joback Method
vc	1.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1862.19	J/mol×K	1224.89	Joback Method
cpg	1917.43	J/mol×K	1270.92	Joback Method
cpg	1976.57	J/mol×K	1316.94	Joback Method
cpg	2040.20	J/mol×K	1362.97	Joback Method
cpg	2108.89	J/mol×K	1409.00	Joback Method
cpg	2183.23	J/mol×K	1455.02	Joback Method
cpg	2263.79	J/mol×K	1501.05	Joback Method

Sources

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=R297537&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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