GA7-3«beta»-O-glucoside, permethylated

Inchi: InChI=1S/C30H42O10/c1-15-12-29-13-16(15)8-9-18(29)30-11-10-19(28(2,27(32)40-30)2
InchiKey: YOYYQLDJKFHNDN-ACYHDOQYSA-N
Formula: C30H42O10
SMILES: C=C1CC23CC1CCC2C12C=CC(OC4OC(COC)C(OC)C(OC)C4OC)C(C)(C(=O)O1)C2C3
Mol. weight [g/mol]: 562.65

Physical Properties

Property code	Value	Unit	Source
gf	-535.43	kJ/mol	Joback Method
hf	-1518.77	kJ/mol	Joback Method
hfus	64.63	kJ/mol	Joback Method
hvap	112.02	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.441		Crippen Method
mcvol	409.900	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
rinpol	3391.00		NIST Webbook
rinpol	3391.00		NIST Webbook
tb	1224.05	K	Joback Method
tc	1499.67	K	Joback Method
tf	879.03	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1827.21	J/mol×K	1224.05	Joback Method
cpg	1882.06	J/mol×K	1269.99	Joback Method
cpg	1940.90	J/mol×K	1315.92	Joback Method
cpg	2004.33	J/mol×K	1361.86	Joback Method
cpg	2072.91	J/mol×K	1407.80	Joback Method
cpg	2147.22	J/mol×K	1453.74	Joback Method
cpg	2227.85	J/mol×K	1499.67	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=R297557&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