

# GA1-3-O-«beta»-D-glucopyranoside, permethyl

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-WWOSSFKKSA-N
Formula:	C31H46O11
SMILES:	C=C1CC23CC1(OC)CCC2C1CCC(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	3580.00		NIST Webbook
rinpol	3580.00		NIST Webbook
rinpol	3580.00		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/molxK	1270.43	Joback Method
cpg	2137.72	J/molxK	1318.74	Joback Method
cpg	2225.40	J/molxK	1367.06	Joback Method
cpg	2321.37	J/molxK	1415.37	Joback Method
cpg	2426.48	J/molxK	1463.68	Joback Method
cpg	2541.58	J/molxK	1512.00	Joback Method
cpg	2667.51	J/molxK	1560.31	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R178951&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R178951&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rlnol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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