

GA5-13-O-«beta»-D-glucopyranoside, permethyl

Other names:	GA5-13-O-glucoside, permethylated
Inchi:	InChI=1S/C30H42O10/c1-16-13-28-15-29(16,39-25-22(36-6)21(35-5)20(34-4)17(38-25)1
InchiKey:	QMGPDYTYPCBFFJ-IYHAUVRDSA-N
Formula:	C30H42O10
SMILES:	C=C1CC23CC1(OC1OC(COC)C(OC)C(OC)C1OC)CCC2C12CC=CC(C)(C(=O)O1)C2C3
Mol. weight [g/mol]:	562.65

Physical Properties

Property code	Value	Unit	Source
gf	-533.21	kJ/mol	Joback Method
hf	-1483.19	kJ/mol	Joback Method
hfus	57.26	kJ/mol	Joback Method
hvap	111.18	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	2.585		Crippen Method
mcvol	409.900	ml/mol	McGowan Method
pc	990.13	kPa	Joback Method
rinpol	3392.00		NIST Webbook
rinpol	3403.00		NIST Webbook
rinpol	3392.00		NIST Webbook
rinpol	3402.00		NIST Webbook
rinpol	3402.00		NIST Webbook
tb	1228.96	K	Joback Method
tc	1504.96	K	Joback Method
tf	907.17	K	Joback Method
vc	1.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1885.66	J/molxK	1228.96	Joback Method
cpg	1958.47	J/molxK	1274.96	Joback Method
cpg	2038.15	J/molxK	1320.96	Joback Method
cpg	2125.47	J/molxK	1366.96	Joback Method

cpg	2221.19	J/mol×K	1412.96	Joback Method
cpg	2326.09	J/mol×K	1458.96	Joback Method
cpg	2440.94	J/mol×K	1504.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R178971&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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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