GA8-2-O-«beta»-D-glucopyranoside, permethyl

Inchi: InChI=1S/C32H48O12/c1-16-12-30-15-31(16,41-9)11-10-19(30)32-13-17(25(39-7)29(2,2

InchiKey: WEKFXKXVNOXNFG-VBHSCQKMSA-N

Formula: C32H48O12

SMILES: C=C1CC23CC1(OC)CCC2C12CC(OC4OC(COC)C(OC)C(OC)C4OC)C(OC)C(C)(C(=O)C

Mol. weight [g/mol]: 624.72

Physical Properties

Property code	Value	Unit	Source
hfus	68.40	kJ/mol	Joback Method
logp	2.059		Crippen Method
mcvol	454.120	ml/mol	McGowan Method
rinpol	3650.00		NIST Webbook
rinpol	3655.00		NIST Webbook
rinpol	3650.00		NIST Webbook

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.26539e+02
Coeff. B	4.20366e+00
Coeff. C	-3.51370e-03
Coeff. D	1.30650e-06
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R178986&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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