GA8-2-O-glucoside, 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-CKAMHMESSA-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
gf	-771.75	kJ/mol	Joback Method
hf	-1887.37	kJ/mol	Joback Method
hfus	65.73	kJ/mol	Joback Method
hvap	119.54	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.059		Crippen Method
mcvol	454.120	ml/mol	McGowan Method
pc	813.53	kPa	Joback Method
rinpol	3650.00		NIST Webbook
rinpol	3652.00		NIST Webbook
rinpol	3658.00		NIST Webbook
tb	1311.06	K	Joback Method
tc	1619.09	K	Joback Method
tf	964.93	K	Joback Method
vc	1.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2194.28	J/mol×K	1311.06	Joback Method
cpg	2282.46	J/mol×K	1362.40	Joback Method
cpg	2378.98	J/mol×K	1413.74	Joback Method
cpg	2484.79	J/mol×K	1465.08	Joback Method
cpg	2600.84	J/mol×K	1516.41	Joback Method
cpg	2728.10	J/mol×K	1567.75	Joback Method
cpg	2867.50	J/mol×K	1619.09	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=R176079&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