

GA8-13-O-glucoside, permethylated

Inchi:	InChI=1S/C32H48O12/c1-16-12-30-15-31(16,43-27-23(39-7)22(38-6)21(37-5)18(42-27)1
InchiKey:	IAPOUDABAQNPNNG-NSTBPJOESA-N
Formula:	C32H48O12
SMILES:	C=C1CC23CC1(OC1OC(COC)C(OC)C(OC)C1OC)CCC2C12CC(OC)C(OC)C(C)(C(=O)O
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	3604.00		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/molxK	1311.06	Joback Method
cpg	2282.46	J/molxK	1362.40	Joback Method
cpg	2378.98	J/molxK	1413.74	Joback Method
cpg	2484.79	J/molxK	1465.08	Joback Method
cpg	2600.84	J/molxK	1516.41	Joback Method
cpg	2728.10	J/molxK	1567.75	Joback Method
cpg	2867.50	J/molxK	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=R297562&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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