GA34-2-O-Glc (17-D2), permethylated

Inchi: InChI=1S/C31H46O11/c1-15-11-30-12-16(15)9-10-19(30)31-13-17(25(38-7)29(2,28(33)4
InchiKey: WJJBZFKBGBQUDT-FOHNHWIVSA-N
Formula: C31H46O11
SMILES: C=C1CC23CC1CCC2C12CC(OC4OC(COC)C(OC)C(OC)C4OC)C(OC)C(C)(C(=O)O1)C
Mol. weight [g/mol]: 594.69

Physical Properties

Property code	Value	Unit	Source
gf	-669.68	kJ/mol	Joback Method
hf	-1749.75	kJ/mol	Joback Method
hfus	68.25	kJ/mol	Joback Method
hvap	116.05	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.290		Crippen Method
mcvol	434.160	ml/mol	McGowan Method
pc	846.03	kPa	Joback Method
rinpol	3532.00		NIST Webbook
rinpol	3534.00		NIST Webbook
rinpol	3534.00		NIST Webbook
tb	1265.52	K	Joback Method
tc	1556.47	K	Joback Method
tf	907.53	K	Joback Method
vc	1.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1983.29	J/mol×K	1265.52	Joback Method
cpg	2042.27	J/mol×K	1314.01	Joback Method
cpg	2105.39	J/mol×K	1362.50	Joback Method
cpg	2173.28	J/mol×K	1410.99	Joback Method
cpg	2246.58	J/mol×K	1459.48	Joback Method
cpg	2325.91	J/mol×K	1507.97	Joback Method
cpg	2411.90	J/mol×K	1556.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R396882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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