Ouabain

Inchi: InChI=1S/C29H44O12/c1-13-22(34)23(35)24(36)25(40-13)41-15-8-19(32)28(12-30)21-1
InchiKey: LPMXVESGRSUGHW-UHFFFAOYSA-N
Formula: C29H44O12
SMILES: CC1OC(OC2CC(O)C3(CO)C4C(O)CC5(C)C(C6=CC(=O)OC6)CCC5(O)C4CCC3(O)C2)C
Mol. weight [g/mol]: 584.65

Physical Properties

Property code	Value	Unit	Source
gf	-1128.61	kJ/mol	Joback Method
hf	-2094.24	kJ/mol	Joback Method
hfus	73.32	kJ/mol	Joback Method
hvap	224.02	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	-1.515		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
tb	1790.71	K	Joback Method
tc	3032.45	K	Joback Method
tf	1189.90	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3563.07	J/mol×K	1790.71	Joback Method
cpg	4693.50	J/mol×K	1997.67	Joback Method
cpg	6236.38	J/mol×K	2204.62	Joback Method
cpg	8268.38	J/mol×K	2411.58	Joback Method
cpg	10866.15	J/mol×K	2618.54	Joback Method
cpg	14106.36	J/mol×K	2825.49	Joback Method
cpg	18065.66	J/mol×K	3032.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6005050&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume