«beta»-Mannosyl-(1-4)-N-acetylglucosamine, permethyl

Inchi: InChI=1S/C21H39NO11/c1-11(23)22-14-17(27-5)16(13(10-25-3)31-20(14)30-8)33-21-19

InchiKey: QOFHGUDPNFUDAH-CQAPXEFUSA-N

Formula: C21H39NO11

SMILES: COCC1OC(OC)C(NC(C)=O)C(OC)C1OC1OC(COC)C(OC)C(OC)C1OC

Mol. weight [g/mol]: 481.53

Physical Properties

Property code	Value	Unit	Source
gf	-938.61	kJ/mol	Joback Method
hf	-1911.72	kJ/mol	Joback Method
hfus	74.54	kJ/mol	Joback Method
hvap	102.21	kJ/mol	Joback Method
log10ws	-0.35		Crippen Method
logp	-0.675		Crippen Method
mcvol	355.280	ml/mol	McGowan Method
pc	997.65	kPa	Joback Method
rinpol	2698.00		NIST Webbook
rinpol	2698.00		NIST Webbook
tb	1018.92	K	Joback Method
tc	1247.65	K	Joback Method
tf	640.84	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.22	J/mol×K	1018.92	Joback Method
cpg	1357.81	J/mol×K	1057.04	Joback Method
cpg	1365.66	J/mol×K	1095.16	Joback Method
cpg	1369.61	J/mol×K	1133.28	Joback Method
cpg	1369.54	J/mol×K	1171.41	Joback Method
cpg	1365.30	J/mol×K	1209.53	Joback Method
cpg	1356.75	J/mol×K	1247.65	Joback Method

Sources

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=R151050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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