«alpha»-D-Glucopyranoside, 1,3,4,6-tetra-O-methyl-«beta»-D-fructofuranosyl 2,3,4,6-tetra-O-methyl-

Other names:	Glucopyranoside, 1,3,4,6-tetra-O-methyl-«beta»-D-fructofuranosyl 2,3,4,6-tetra-O-methyl, «alpha»-D- Octa-O-methylsucrose Permethyl sucrose Glucopyranoside, 1,3,4,6-tetra-O-methyl-«beta»-D-fructofuranosyl 2,3,4,6-tetra-O-methyl- Sucrose, permethyl
Inchi:	InChI=1S/C20H38O11/c1-21-9-12-14(24-4)16(26-6)17(27-7)19(29-12)31-20(11-23-3)18(
InchiKey:	RNUOORAGNGKJLZ-PBNBPITBSA-N
Formula:	C20H38O11
SMILES:	COCC1OC(OC2(COC)OC(COC)C(OC)C2OC)C(OC)C(OC)C1OC
Mol. weight [g/mol]:	454.51
CAS:	5346-73-6

Physical Properties

Property code	Value	Unit	Source
gf	-998.18	kJ/mol	Joback Method
hf	-1922.45	kJ/mol	Joback Method
hfus	61.17	kJ/mol	Joback Method
hvap	88.20	kJ/mol	Joback Method
log10ws	0.06		Crippen Method
logp	-0.163		Crippen Method
mcvol	335.510	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
tb	915.06	K	Joback Method
tc	1122.53	K	Joback Method
tf	580.87	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1230.40	J/mol×K	915.06	Joback Method
cpg	1251.53	J/mol×K	949.64	Joback Method
cpg	1270.82	J/mol×K	984.22	Joback Method
cpg	1288.23	J/mol×K	1018.80	Joback Method

cpg	1303.72	J/mol×K	1053.38	Joback Method
cpg	1317.27	J/mol×K	1087.95	Joback Method
cpg	1328.84	J/mol×K	1122.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5346736&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