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

Other names: Glucopyranoside, 1,3,4,6-tetra-O-methyl-«beta»-D-fructofuranosyl 2,3,4-tri-O-methyl-6-O-(2,3,4,6-tetra-O-methyl-«alpha»-D-galactopyranosyl-(1->6)-«alpha»-D-; Raffinose, permethyl

Inchi: InChI=1S/C29H54O16/c1-30-12-16-19(33-4)22(36-7)24(38-9)27(42-16)41-14-17-20(34-5

InchiKey: CODTYWQHUHJXKQ-UHFQAHCESA-N

Formula: C29H54O16

SMILES: COCC1OC(OCC2OC(OC3(COC)OC(COC)C(OC)C3OC)C(OC)C(OC)C2OC)C(OC)C(OC

Mol. weight [g/mol]: 658.73

CAS: 34141-00-9

Physical Properties

Property code	Value	Unit	Source
gf	-1434.91	kJ/mol	Joback Method
hf	-2796.13	kJ/mol	Joback Method
hfus	93.34	kJ/mol	Joback Method
hvap	121.57	kJ/mol	Joback Method
log10ws	-0.09		Crippen Method
logp	-0.376		Crippen Method
mcvol	480.810	ml/mol	McGowan Method
pc	631.93	kPa	Joback Method
tb	1238.48	K	Joback Method
tc	1564.55	K	Joback Method
tf	788.21	K	Joback Method
vc	1.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1925.65	J/mol×K	1238.48	Joback Method
cpg	1918.61	J/mol×K	1292.82	Joback Method
cpg	1901.70	J/mol×K	1347.17	Joback Method
cpg	1874.59	J/mol×K	1401.51	Joback Method
cpg	1836.91	J/mol×K	1455.86	Joback Method
cpg	1788.33	J/mol×K	1510.20	Joback Method
cpg	1728.51	J/mol×K	1564.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34141009&Units=SI

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