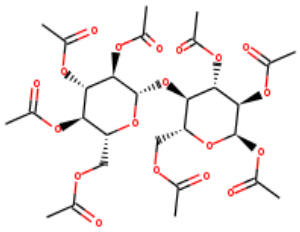
«alpha»-D-Cellobiose octaacetate



Other names: Cellobiose octaacetate; Cellobiose, octaacetate alpha, d-; Cellobiose, octaacetate, «alpha»-; Cellobiose, octaacetate, «alpha»-D-; D-Cellobiose octaacetate; Octaacetyl-«alpha»-cellobiose; alpha-D-Cellobiose octaacetate; «alpha»-D-Glucopyranose, 4-O-(2,3,4,6-tetra-O-acetyl-«beta»-D-glucopyranosyl)-, tetraacetate.

InChI: InChI=1S/C28H38O19/c1-11(29)37-9-19-21(39-13(3)31)23(40-14(4)32)26(43-17(7)35)28(46-19)47-22-20(10-38-12(2)30)45-27(44-18(8)36)25(42-16(6)34)24(22)41-15(5)33/h19-28H,9-10H2,1-8H3/t19-,20-,21-,22-,23+,24+,25-,26-,27+,28+/m0/s1

InChI Key: WOTQVEKSRLZRSX-GCUFADGCSA-N

Formula: C28H38O19

SMILES: CC(=O)OCC1OC(OC2C(COC(C)=O)OC(OC(C)=O)C(OC(C)=O)C2OC(C)=O)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O

Molecular Weight: 678.59

CAS: 5346-90-7

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-1976.50	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-3029.95	kJ/mol	Joback Method
$\Delta_{fus} H°$	99.96	kJ/mol	Joback Method
$\Delta_{vap} H°$	160.99	kJ/mol	Joback Method
$logP_{oct/wat}$	-0.831		Crippen Method
P_c	851.47	kPa	Joback Method
T_{boil}	1528.42	K	Joback Method
T_c	2047.08	K	Joback Method
T_{fus}	1038.81	K	Joback Method
V_c	1.714	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1350.50	J/mol×K	1528.42	Joback Method

Property	Value	Unit	Temperature (K)	Source
η	0.0000112	Pa×s	1528.42	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C28H38O19/c1-11(29)37-9-19-21(39-13(3)31)23(40-14(4)32)26(43-17(7)35)28(46-19)47-22-20(10-38-12(2)30)45-27(44-18(8)36)25(42-16(6)34)24(22)41-15(5)33/h19-28H,9-10H2,1-8H3/t19-,20-,21-,22-,23+,24+,25-,26-,27+,28+/m0/s1

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: Enthalpy of vaporization at standard conditions (kJ/mol).
$logP_{oct/wat}$: Octanol/Water partition coefficient .
P_c: Critical Pressure (kPa).
T_{boil}: Normal Boiling Point Temperature (K).
T_c: Critical Temperature (K).
T_{fus}: Normal melting (fusion) point (K).
V_c: Critical Volume (m^3/kg-mol).