«alpha»-D-Cellobiose octaacetate

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

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

InchiKey: 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

Mol. weight [g/mol]: 678.59

CAS: 5346-90-7

Physical Properties

Property code	Value	Unit	Source
gf	-1976.50	kJ/mol	Joback Method
hf	-3029.95	kJ/mol	Joback Method
hfus	99.96	kJ/mol	Joback Method
hvap	160.99	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	-0.831		Crippen Method
mcvol	460.790	ml/mol	McGowan Method
pc	851.47	kPa	Joback Method
tb	1528.42	K	Joback Method
tc	2047.08	K	Joback Method
tf	1038.81	K	Joback Method
vc	1.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1350.50	J/mol×K	1528.42	Joback Method

cpg	1203.74	J/mol×K	1614.86	Joback Method
cpg	1022.51	J/mol×K	1701.31	Joback Method
cpg	805.02	J/mol×K	1787.75	Joback Method
cpg	549.44	J/mol×K	1874.19	Joback Method
cpg	253.97	J/mol×K	1960.64	Joback Method
cpg	-83.21	J/mol×K	2047.08	Joback Method
dvisc	0.0000481	Pa×s	1038.81	Joback Method
dvisc	0.0000345	Pa×s	1120.41	Joback Method
dvisc	0.0000259	Pa×s	1202.01	Joback Method
dvisc	0.0000201	Pa×s	1283.62	Joback Method
dvisc	0.0000162	Pa×s	1365.22	Joback Method
dvisc	0.0000133	Pa×s	1446.82	Joback Method
dvisc	0.0000112	Pa×s	1528.42	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=C5346907&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
dvisc: Dynamic viscosity
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