

D-Glucose, 2,3,4,5,6-pentaacetate

Other names:	D-Glucose pentaacetate Glucose pentaacetate Pentaacetylglucose «alpha»-d-Glucose 2,3,4,5,6-pentaacetate d-Allose, pentaacetate (ester) Glucose acetate
Inchi:	InChI=1S/C16H22O11/c1-8(18)23-7-14(25-10(3)20)16(27-12(5)22)15(26-11(4)21)13(6-1
InchiKey:	UAOKXEHOENRFMP-UHFFFAOYSA-N
Formula:	C16H22O11
SMILES:	CC(=O)OCC(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C(C=O)OC(C)=O
Mol. weight [g/mol]:	390.34
CAS:	3891-59-6

Physical Properties

Property code	Value	Unit	Source
chs	-7190.90 ± 1.60	kJ/mol	NIST Webbook
gf	-1195.04	kJ/mol	Joback Method
hf	-1704.27	kJ/mol	Joback Method
hfs	-2249.40 ± 1.70	kJ/mol	NIST Webbook
hfus	39.33	kJ/mol	Joback Method
hvap	102.16	kJ/mol	Joback Method
log10ws	-0.56		Crippen Method
logp	-0.525		Crippen Method
mcvol	275.070	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	2010.00		NIST Webbook
tb	993.83	K	Joback Method
tc	1217.09	K	Joback Method
tf	612.88	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
---------------	-------	------	-----------------	--------

cpg	873.89	J/molxK	993.83	Joback Method
cpg	881.71	J/molxK	1031.04	Joback Method
cpg	887.72	J/molxK	1068.25	Joback Method
cpg	891.89	J/molxK	1105.46	Joback Method
cpg	894.17	J/molxK	1142.67	Joback Method
cpg	894.52	J/molxK	1179.88	Joback Method
cpg	892.89	J/molxK	1217.09	Joback Method
dvisc	0.0002906	Paxs	612.88	Joback Method
dvisc	0.0001574	Paxs	676.37	Joback Method
dvisc	0.0000947	Paxs	739.86	Joback Method
dvisc	0.0000618	Paxs	803.36	Joback Method
dvisc	0.0000429	Paxs	866.85	Joback Method
dvisc	0.0000313	Paxs	930.34	Joback Method
dvisc	0.0000238	Paxs	993.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3891596&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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

Latest version available from:

<https://www.cheméo.com/cid/14-647-8/D-Glucose-2-3-4-5-6-pentaacetate.pdf>

Generated by Cheméo on 2024-04-19 22:38:06.242493703 +0000 UTC m=+15855535.163071018.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.