

1,5-Anhydro-2,3,4,6-tetra-O-methyl-D-glucitol

Inchi:	InChI=1S/C10H20O5/c1-11-5-8-10(14-4)9(13-3)7(12-2)6-15-8/h7-10H,5-6H2,1-4H3/t7-,8
InchiKey:	SQOPNOVHKFZFPJ-IMSYWVGJSA-N
Formula:	C10H20O5
SMILES:	COCC1OCC(OC)C(OC)C1OC
Mol. weight [g/mol]:	220.26
CAS:	81874-02-4

Physical Properties

Property code	Value	Unit	Source
gf	-471.48	kJ/mol	Joback Method
hf	-917.31	kJ/mol	Joback Method
hfus	29.44	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
log10ws	0.21		Crippen Method
logp	0.077		Crippen Method
mcvol	170.250	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1363.28		NIST Webbook
rinpol	1363.28		NIST Webbook
tb	550.37	K	Joback Method
tc	740.59	K	Joback Method
tf	312.61	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.39	J/molxK	550.37	Joback Method
cpg	532.40	J/molxK	708.89	Joback Method
cpg	516.82	J/molxK	677.18	Joback Method
cpg	500.50	J/molxK	645.48	Joback Method
cpg	483.46	J/molxK	613.78	Joback Method
cpg	465.74	J/molxK	582.07	Joback Method
cpg	547.18	J/molxK	740.59	Joback Method

dvisc	0.0001628	Paxs	550.37	Joback Method
dvisc	0.0001969	Paxs	510.74	Joback Method
dvisc	0.0002458	Paxs	471.12	Joback Method
dvisc	0.0003197	Paxs	431.49	Joback Method
dvisc	0.0004386	Paxs	391.86	Joback Method
dvisc	0.0006459	Paxs	352.24	Joback Method
dvisc	0.0010494	Paxs	312.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81874024&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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