1,4:3,6-Dianhydro-«alpha»-d-glucopyranose

Other names: 1.4:3,6-Dianhydro-A-D-glucopyranose
Inchi: InChI=1S/C6H8O4/c7-3-5-4-2(1-8-5)9-6(3)10-4/h2-7H,1H2/t2-,3-,4-,5-,6+/m0/s1
InchiKey: XOTJGHCMZOLIPX-GKFJPSPNSA-N
Formula: C6H8O4
SMILES: OC1C2OC3COC1C3O2
Mol. weight [g/mol]: 144.13

Physical Properties

Property code	Value	Unit	Source
gf	-228.71	kJ/mol	Joback Method
hf	-537.68	kJ/mol	Joback Method
hfus	35.87	kJ/mol	Joback Method
hvap	58.28	kJ/mol	Joback Method
log10ws	0.40		Crippen Method
logp	-1.130		Crippen Method
mcvol	86.300	ml/mol	McGowan Method
pc	5065.79	kPa	Joback Method
ripol	2394.00		NIST Webbook
ripol	2394.00		NIST Webbook
tb	520.59	K	Joback Method
tc	721.10	K	Joback Method
tf	343.25	K	Joback Method
vc	0.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.97	J/mol×K	520.59	Joback Method
cpg	297.54	J/mol×K	687.68	Joback Method
cpg	289.01	J/mol×K	654.26	Joback Method
cpg	279.85	J/mol×K	620.84	Joback Method
cpg	270.00	J/mol×K	587.43	Joback Method
cpg	259.39	J/mol×K	554.01	Joback Method
cpg	305.51	J/mol×K	721.10	Joback Method

dvisc	0.0017956	Pa×s	520.59	Joback Method
dvisc	0.0020707	Pa×s	491.03	Joback Method
dvisc	0.0024318	Pa×s	461.48	Joback Method
dvisc	0.0029196	Pa×s	431.92	Joback Method
dvisc	0.0036006	Pa×s	402.36	Joback Method
dvisc	0.0045905	Pa×s	372.81	Joback Method
dvisc	0.0061025	Pa×s	343.25	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=U98148&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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