2,3-dihydro-3,5-dihydroxy-4H-pyran-4-one

Inchi: InChI=1S/C5H6O4/c6-3-1-9-2-4(7)5(3)8/h1,4,6-7H,2H2
InchiKey: QVQTZFXVGAPBRV-UHFFFAOYSA-N
Formula: C5H6O4
SMILES: O=C1C(O)=COCC1O
Mol. weight [g/mol]: 130.10

Physical Properties

Property code	Value	Unit	Source
gf	-446.35	kJ/mol	Joback Method
hf	-620.06	kJ/mol	Joback Method
hfus	17.04	kJ/mol	Joback Method
hvap	70.22	kJ/mol	Joback Method
log10ws	0.28		Crippen Method
logp	-0.654		Crippen Method
mcvol	85.330	ml/mol	McGowan Method
pc	6278.87	kPa	Joback Method
rinpol	1167.00		NIST Webbook
rinpol	1167.00		NIST Webbook
tb	616.62	K	Joback Method
tc	818.23	K	Joback Method
tf	383.20	K	Joback Method
vc	0.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.64	J/mol×K	616.62	Joback Method
cpg	227.63	J/mol×K	650.22	Joback Method
cpg	235.21	J/mol×K	683.82	Joback Method
cpg	242.37	J/mol×K	717.42	Joback Method
cpg	249.10	J/mol×K	751.03	Joback Method
cpg	255.38	J/mol×K	784.63	Joback Method
cpg	261.20	J/mol×K	818.23	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=R231037&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
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