4-Hydroxy-5,6-dihydro-2H-pyran-2-one

Inchi: InChI=1S/C5H6O3/c6-4-1-2-8-5(7)3-4/h3,6H,1-2H2
InchiKey: NJGFHHXZSDLYQJ-UHFFFAOYSA-N
Formula: C5H6O3
SMILES: O=C1C=C(O)CCO1
Mol. weight [g/mol]: 114.10

Physical Properties

Property code	Value	Unit	Source
gf	-301.82	kJ/mol	Joback Method
hf	-447.49	kJ/mol	Joback Method
hfus	11.88	kJ/mol	Joback Method
hvap	53.85	kJ/mol	Joback Method
log10ws	-0.35		Crippen Method
logp	0.375		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	5730.52	kPa	Joback Method
rinpol	1004.00		NIST Webbook
rinpol	1004.00		NIST Webbook
ripol	1842.00		NIST Webbook
ripol	1842.00		NIST Webbook
tb	529.11	K	Joback Method
tc	745.84	K	Joback Method
tf	326.62	K	Joback Method
vc	0.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.58	J/mol×K	529.11	Joback Method
cpg	186.55	J/mol×K	565.23	Joback Method
cpg	195.11	J/mol×K	601.35	Joback Method
cpg	203.24	J/mol×K	637.47	Joback Method
cpg	210.95	J/mol×K	673.59	Joback Method
cpg	218.20	J/mol×K	709.71	Joback Method

cpg	225.00	J/mol×K	745.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R318664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume