2,3-Dihydro-5-hydroxy-6-methyl-4H-pyran-4-one

Inchi: InChI=1S/C6H8O3/c1-4-6(8)5(7)2-3-9-4/h8H,2-3H2,1H3
InchiKey: YTKBKDDTNVNZLX-UHFFFAOYSA-N
Formula: C6H8O3
SMILES: CC1=C(O)C(=O)CCO1
Mol. weight [g/mol]: 128.13

Physical Properties

Property code	Value	Unit	Source
gf	-303.03	kJ/mol	Joback Method
hf	-479.60	kJ/mol	Joback Method
hfus	14.08	kJ/mol	Joback Method
hvap	56.74	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method
logp	0.765		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	4876.56	kPa	Joback Method
rinpol	1103.00		NIST Webbook
rinpol	1103.00		NIST Webbook
tb	556.97	K	Joback Method
tc	771.16	K	Joback Method
tf	350.41	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.38	J/mol×K	556.97	Joback Method
cpg	229.26	J/mol×K	592.67	Joback Method
cpg	238.71	J/mol×K	628.37	Joback Method
cpg	247.70	J/mol×K	664.06	Joback Method
cpg	256.23	J/mol×K	699.76	Joback Method
cpg	264.27	J/mol×K	735.46	Joback Method
cpg	271.82	J/mol×K	771.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R612530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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