4H-Pyran-4-one, 2,3-dihydro-3-hydroxy-6-formyl

Inchi: InChI=1S/C6H6O4/c7-2-4-1-5(8)6(9)3-10-4/h1-2,6,9H,3H2

InchiKey: MOGMYZWZFVCQNF-UHFFFAOYSA-N

Formula: C6H6O4

SMILES: O=CC1=CC(=O)C(O)CO1

Mol. weight [g/mol]: 142.11

Physical Properties

Property code	Value	Unit	Source
gf	-400.63	kJ/mol	Joback Method
hf	-574.05	kJ/mol	Joback Method
hfus	17.83	kJ/mol	Joback Method
hvap	62.49	kJ/mol	Joback Method
log10ws	0.40		Crippen Method
logp	-0.971		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
tb	595.98	K	Joback Method
tc	811.86	K	Joback Method
tf	375.65	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.86	J/mol×K	595.98	Joback Method
cpg	244.18	J/mol×K	631.96	Joback Method
cpg	253.01	J/mol×K	667.94	Joback Method
cpg	261.31	J/mol×K	703.92	Joback Method
cpg	269.08	J/mol×K	739.90	Joback Method
cpg	276.30	J/mol×K	775.88	Joback Method
cpg	282.95	J/mol×K	811.86	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=R74668&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