Dihydro-5-(hydroxymethyl)-2(3H)-furanone

Inchi: InChI=1S/C5H6O3/c6-3-4-1-2-5(7)8-4/h1,6H,2-3H2
InchiKey: IPNRODMULRDGPT-UHFFFAOYSA-N
Formula: C5H6O3
SMILES: O=C1CC=C(CO)O1
Mol. weight [g/mol]: 114.10

Physical Properties

Property code	Value	Unit	Source
gf	-289.72	kJ/mol	Joback Method
hf	-441.33	kJ/mol	Joback Method
hfus	13.98	kJ/mol	Joback Method
hvap	53.68	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	-0.191		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	5519.63	kPa	Joback Method
ripol	2516.00		NIST Webbook
tb	524.84	K	Joback Method
tc	733.86	K	Joback Method
tf	330.14	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.20	J/mol×K	524.84	Joback Method
cpg	186.40	J/mol×K	559.68	Joback Method
cpg	194.23	J/mol×K	594.51	Joback Method
cpg	201.69	J/mol×K	629.35	Joback Method
cpg	208.77	J/mol×K	664.19	Joback Method
cpg	215.47	J/mol×K	699.03	Joback Method
cpg	221.79	J/mol×K	733.86	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R591047&Units=SI

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