(S)-5-Hydroxymethyl-2[5H]-furanone

Inchi: InChI=1S/C5H6O3/c6-3-4-1-2-5(7)8-4/h1-2,4,6H,3H2/t4-/m1/s1
InchiKey: AWNLUIGMHSSXHB-SCSAIBSYSA-N
Formula: C5H6O3
SMILES: O=C1C=CC(CO)O1
Mol. weight [g/mol]: 114.10
CAS: 78508-96-0

Physical Properties

Property code	Value	Unit	Source
gf	-287.80	kJ/mol	Joback Method
hf	-450.20	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	52.71	kJ/mol	Joback Method
log10ws	0.10		Crippen Method
logp	-0.540		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	5374.91	kPa	Joback Method
tb	515.19	K	Joback Method
tc	722.90	K	Joback Method
tf	313.38	K	Joback Method
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.96	J/mol×K	515.19	Joback Method
cpg	189.83	J/mol×K	549.81	Joback Method
cpg	198.29	J/mol×K	584.43	Joback Method
cpg	206.35	J/mol×K	619.05	Joback Method
cpg	213.99	J/mol×K	653.66	Joback Method
cpg	221.21	J/mol×K	688.28	Joback Method
cpg	228.01	J/mol×K	722.90	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=C78508960&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume