

5-(1-Hydroxyethyl)-2(3H)-furanone, solerol isomer

Other names:	Dihydro-5-(1-hydroxyethyl)-2(3H)-furanone
Inchi:	InChI=1S/C6H8O3/c1-4(7)5-2-3-6(8)9-5/h2,4,7H,3H2,1H3
InchiKey:	SJEIEJGZIWPGFN-UHFFFAOYSA-N
Formula:	C6H8O3
SMILES:	CC(O)C1=CCC(=O)O1
Mol. weight [g/mol]:	128.13

Physical Properties

Property code	Value	Unit	Source
gf	-283.74	kJ/mol	Joback Method
hf	-467.25	kJ/mol	Joback Method
hfus	13.05	kJ/mol	Joback Method
hvap	55.52	kJ/mol	Joback Method
log10ws	-0.82		Crippen Method
logp	0.198		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	4862.97	kPa	Joback Method
ripol	2378.00		NIST Webbook
ripol	2343.00		NIST Webbook
ripol	2345.00		NIST Webbook
ripol	2343.00		NIST Webbook
ripol	2378.00		NIST Webbook
tb	547.28	K	Joback Method
tc	757.55	K	Joback Method
tf	326.41	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.78	J/molxK	547.28	Joback Method
cpg	230.43	J/molxK	582.32	Joback Method
cpg	239.61	J/molxK	617.37	Joback Method
cpg	248.32	J/molxK	652.41	Joback Method

cpg	256.56	J/mol×K	687.46	Joback Method
cpg	264.33	J/mol×K	722.50	Joback Method
cpg	271.62	J/mol×K	757.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R513458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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