2,5-Dimethyl-3-(1-hydroxyethyl)-furan

Inchi: InChI=1S/C9H14O/c1-6-4-7(2)9(5-6)8(3)10/h5,8,10H,4H2,1-3H3
InchiKey: QHIRFADJWIMMHP-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CC1=CC(C(C)O)=C(C)C1
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
gf	-39.07	kJ/mol	Joback Method
hf	-224.63	kJ/mol	Joback Method
hfus	13.77	kJ/mol	Joback Method
hvap	55.05	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.034		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
rinpol	1196.00		NIST Webbook
tb	530.27	K	Joback Method
tc	722.92	K	Joback Method
tf	291.23	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.56	J/mol×K	530.27	Joback Method
cpg	296.25	J/mol×K	562.38	Joback Method
cpg	307.37	J/mol×K	594.49	Joback Method
cpg	317.94	J/mol×K	626.59	Joback Method
cpg	327.99	J/mol×K	658.70	Joback Method
cpg	337.53	J/mol×K	690.81	Joback Method
cpg	346.59	J/mol×K	722.92	Joback Method
dvisc	0.0091403	Pa×s	291.23	Joback Method
dvisc	0.0029601	Pa×s	331.07	Joback Method

dvisc	0.0012214	Pa×s	370.91	Joback Method
dvisc	0.0005984	Pa×s	410.75	Joback Method
dvisc	0.0003326	Pa×s	450.59	Joback Method
dvisc	0.0002034	Pa×s	490.43	Joback Method
dvisc	0.0001339	Pa×s	530.27	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R440429&Units=SI

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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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