2-(1-hydroxyethyl)-4,5-dihydrothiazole

Inchi: InChI=1S/C5H9NOS/c1-4(7)5-6-2-3-8-5/h4,7H,2-3H2,1H3
InchiKey: IOZOUUUQYPXUAJ-UHFFFAOYSA-N
Formula: C5H9NOS
SMILES: CC(O)C1=NCCS1
Mol. weight [g/mol]: 131.20

Physical Properties

Property code	Value	Unit	Source
gf	73.19	kJ/mol	Joback Method
hf	-60.68	kJ/mol	Joback Method
hfus	11.76	kJ/mol	Joback Method
hvap	56.56	kJ/mol	Joback Method
log10ws	-0.73		Crippen Method
logp	0.512		Crippen Method
mcvol	98.350	ml/mol	McGowan Method
pc	5335.72	kPa	Joback Method
ripol	1909.00		NIST Webbook
tb	531.16	K	Joback Method
tc	752.58	K	Joback Method
tf	375.34	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.22	J/mol×K	531.16	Joback Method
cpg	236.14	J/mol×K	568.06	Joback Method
cpg	246.41	J/mol×K	604.97	Joback Method
cpg	256.05	J/mol×K	641.87	Joback Method
cpg	265.06	J/mol×K	678.77	Joback Method
cpg	273.47	J/mol×K	715.68	Joback Method
cpg	281.30	J/mol×K	752.58	Joback Method

Sources

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=R334686&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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