

2-methyl-4,5-dihydrofuran-5-spiro-2'-thiazolidine

Inchi:	InChI=1S/C7H11NOS/c1-6-2-3-7(9-6)8-4-5-10-7/h2,8H,3-5H2,1H3
InchiKey:	JSUHZHHHAKHBNL-UHFFFAOYSA-N
Formula:	C7H11NOS
SMILES:	CC1=CCC2(NCCS2)O1
Mol. weight [g/mol]:	157.23

Physical Properties

Property code	Value	Unit	Source
gf	157.26	kJ/mol	Joback Method
hf	-27.73	kJ/mol	Joback Method
hfus	18.55	kJ/mol	Joback Method
hvap	48.71	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.301		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	518.23	K	Joback Method
tc	776.91	K	Joback Method
tf	450.44	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.96	J/molxK	518.23	Joback Method
cpg	274.64	J/molxK	561.34	Joback Method
cpg	288.03	J/molxK	604.46	Joback Method
cpg	300.35	J/molxK	647.57	Joback Method
cpg	311.82	J/molxK	690.69	Joback Method
cpg	322.65	J/molxK	733.80	Joback Method
cpg	333.07	J/molxK	776.91	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=R321536&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

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