2-methyltetrahydrofuran-3-spiro-2'-thiazolidine

Inchi: InChI=1S/C7H13NOS/c1-6-7(2-4-9-6)8-3-5-10-7/h6,8H,2-5H2,1H3
InchiKey: OPFPLXAEUOBWQR-UHFFFAOYSA-N
Formula: C7H13NOS
SMILES: CC1OCCC12NCCS2
Mol. weight [g/mol]: 159.25

Physical Properties

Property code	Value	Unit	Source
gf	129.22	kJ/mol	Joback Method
hf	-94.38	kJ/mol	Joback Method
hfus	18.78	kJ/mol	Joback Method
hvap	47.45	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	0.828		Crippen Method
mcvol	119.970	ml/mol	McGowan Method
pc	4444.44	kPa	Joback Method
ripol	2024.00		NIST Webbook
tb	509.42	K	Joback Method
tc	763.97	K	Joback Method
tf	432.92	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.66	J/mol×K	509.42	Joback Method
cpg	295.82	J/mol×K	551.85	Joback Method
cpg	311.54	J/mol×K	594.27	Joback Method
cpg	326.05	J/mol×K	636.70	Joback Method
cpg	339.53	J/mol×K	679.12	Joback Method
cpg	352.20	J/mol×K	721.55	Joback Method
cpg	364.27	J/mol×K	763.97	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=R321541&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