

4-Hydroxy-4,5,5-trimethylthiazolidine-2-thione

Inchi:	InChI=1S/C6H11NOS2/c1-5(2)6(3,8)7-4(9)10-5/h8H,1-3H3,(H,7,9)
InchiKey:	CFUUNLSMDIFGY-UHFFFAOYSA-N
Formula:	C6H11NOS2
SMILES:	CC1(O)NC(=S)SC1(C)C
Mol. weight [g/mol]:	177.29
CAS:	19975-64-5

Physical Properties

Property code	Value	Unit	Source
gf	99.10	kJ/mol	Joback Method
hf	-50.61	kJ/mol	Joback Method
hfus	17.07	kJ/mol	Joback Method
hvap	63.32	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	1.095		Crippen Method
mcvol	128.790	ml/mol	McGowan Method
pc	5235.81	kPa	Joback Method
tb	608.97	K	Joback Method
tc	849.84	K	Joback Method
tf	524.81	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.96	J/molxK	608.97	Joback Method
cpg	306.51	J/molxK	649.11	Joback Method
cpg	315.61	J/molxK	689.26	Joback Method
cpg	324.54	J/molxK	729.40	Joback Method
cpg	333.59	J/molxK	769.55	Joback Method
cpg	343.03	J/molxK	809.69	Joback Method
cpg	353.13	J/molxK	849.84	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=C19975645&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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