

Spiro(1,2-dithiolane-4,5'-hydantoin)

Inchi:	InChI=1S/C5H6N2O2S2/c8-3-5(1-10-11-2-5)7-4(9)6-3/h1-2H2,(H2,6,7,8,9)
InchiKey:	DPGBTPQJLUGDOZ-UHFFFAOYSA-N
Formula:	C5H6N2O2S2
SMILES:	O=C1NC(=O)C2(CSSC2)N1
Mol. weight [g/mol]:	190.24
CAS:	62032-12-6

Physical Properties

Property code	Value	Unit	Source
gf	88.60	kJ/mol	Joback Method
hf	-93.09	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	59.86	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	-0.040		Crippen Method
mcvol	115.390	ml/mol	McGowan Method
pc	7218.50	kPa	Joback Method
tb	673.40	K	Joback Method
tc	992.27	K	Joback Method
tf	712.97	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.68	J/molxK	673.40	Joback Method
cpg	293.04	J/molxK	726.55	Joback Method
cpg	305.79	J/molxK	779.69	Joback Method
cpg	318.10	J/molxK	832.84	Joback Method
cpg	330.17	J/molxK	885.98	Joback Method
cpg	342.19	J/molxK	939.13	Joback Method
cpg	354.34	J/molxK	992.27	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=C62032126&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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