2-Pyrrolidinethione

Other names:	«gamma»-Butyrothiolactam
	Thiobutyrolactam
	Thiopyrrolidone
	2-Pyrrolethione, tetrahydro-,
	Tetrahydro-2-pyrrolethione
Inchi:	InChI=1S/C4H7NS/c6-4-2-1-3-5-4/h1-3H2,(H,5,6)
InchiKey:	IMWUREPEYPRYOR-UHFFFAOYSA-N
Formula:	C4H7NS
SMILES:	S=C1CCCN1
Mol. weight [g/mol]:	101.17
CAS:	2295-35-4

Physical Properties

Property code	Value	Unit	Source
gf	205.62	kJ/mol	Joback Method
hf	107.84	kJ/mol	Joback Method
hfus	14.60	kJ/mol	Joback Method
hvap	39.30	kJ/mol	Joback Method
ie	8.14	eV	NIST Webbook
log10ws	-1.43		Crippen Method
logp	0.697		Crippen Method
mcvol	78.390	ml/mol	McGowan Method
pc	5917.16	kPa	Joback Method
tb	432.06	K	Joback Method
tc	668.83	K	Joback Method
tf	318.68	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.77	J/mol×K	432.06	Joback Method
cpg	143.54	J/mol×K	471.52	Joback Method
cpg	152.60	J/mol×K	510.98	Joback Method

cpg	161.01	J/mol×K	550.45	Joback Method
cpg	168.81	J/mol×K	589.91	Joback Method
cpg	176.04	J/mol×K	629.37	Joback Method
cpg	182.75	J/mol×K	668.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2295354&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ie:	Ionization energy
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