

Rhodanine, 5-cyclohexylidene-

Inchi:	InChI=1S/C9H11NOS2/c11-8-7(13-9(12)10-8)6-4-2-1-3-5-6/h1-5H2,(H,10,11,12)
InchiKey:	GFDLUSAUGSDHAD-UHFFFAOYSA-N
Formula:	C9H11NOS2
SMILES:	O=C1NC(=S)SC1=C1CCCCC1
Mol. weight [g/mol]:	213.32
CAS:	3698-06-4

Physical Properties

Property code	Value	Unit	Source
gf	207.85	kJ/mol	Joback Method
hf	21.70	kJ/mol	Joback Method
hfus	21.93	kJ/mol	Joback Method
hvap	62.84	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	2.353		Crippen Method
mcvol	151.600	ml/mol	McGowan Method
pc	4403.25	kPa	Joback Method
tb	695.45	K	Joback Method
tc	986.48	K	Joback Method
tf	564.12	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.30	J/molxK	695.45	Joback Method
cpg	390.37	J/molxK	743.95	Joback Method
cpg	404.15	J/molxK	792.46	Joback Method
cpg	416.69	J/molxK	840.96	Joback Method
cpg	428.05	J/molxK	889.47	Joback Method
cpg	438.27	J/molxK	937.97	Joback Method
cpg	447.41	J/molxK	986.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3698064&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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