

Rhodanine, 5-p-hydroxybenzylidene-

Inchi:	InChI=1S/C10H7NO2S2/c12-7-3-1-6(2-4-7)5-8-9(13)11-10(14)15-8/h1-5,12H,(H,11,13,14)
InchiKey:	RAYIDZVPIAJJPF-YVMONPNESA-N
Formula:	C10H7NO2S2
SMILES:	O=C1NC(=S)SC1=Cc1ccc(O)cc1
Mol. weight [g/mol]:	237.30
CAS:	6339-79-3

Physical Properties

Property code	Value	Unit	Source
gf	176.66	kJ/mol	Joback Method
hf	26.81	kJ/mol	Joback Method
hfus	33.46	kJ/mol	Joback Method
hvap	78.79	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	1.881		Crippen Method
mcvol	158.660	ml/mol	McGowan Method
pc	5585.83	kPa	Joback Method
tb	798.93	K	Joback Method
tc	1099.60	K	Joback Method
tf	686.47	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.56	J/molxK	798.93	Joback Method
cpg	401.12	J/molxK	849.04	Joback Method
cpg	411.10	J/molxK	899.15	Joback Method
cpg	420.71	J/molxK	949.26	Joback Method
cpg	430.12	J/molxK	999.37	Joback Method
cpg	439.54	J/molxK	1049.49	Joback Method
cpg	449.16	J/molxK	1099.60	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6339793&Units=SI

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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