

4-Thiazolidinone, 5-(p-hydroxybenzylidene)-2-imino-

Inchi:	InChI=1S/C10H8N2O2S/c11-10-12-9(14)8(15-10)5-6-1-3-7(13)4-2-6/h1-5,13H,(H2,11,12)
InchiKey:	YBHQ CJILTOVLHD-VMPITWQZSA-N
Formula:	C10H8N2O2S
SMILES:	<chem>N=C1NC(=O)C(=Cc2ccc(O)cc2)S1</chem>
Mol. weight [g/mol]:	220.25
CAS:	299953-00-7

Physical Properties

Property code	Value	Unit	Source
gf	263.20	kJ/mol	Joback Method
hf	78.64	kJ/mol	Joback Method
hvap	84.14	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	1.531		Crippen Method
mvol	152.290	ml/mol	McGowan Method
tb	813.23	K	Joback Method
tf	720.98	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.09	J/molxK	813.23	Joback Method
cpg	63.23	J/molxK	100.12	Joback Method
cpg	63.23	J/molxK	100.12	Joback Method
cpg	63.23	J/molxK	100.12	Joback Method
cpg	63.23	J/molxK	100.12	Joback Method
cpg	63.23	J/molxK	100.12	Joback Method
cpg	63.23	J/molxK	100.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C299953007&Units=SI
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

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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