

4-Thiazolidinone, 5-benzylidene-2-imino-

Inchi:	InChI=1S/C10H8N2OS/c11-10-12-9(13)8(14-10)6-7-4-2-1-3-5-7/h1-6H,(H2,11,12,13)/b8-
InchiKey:	SRILECHSVYTLLS-SOFGYWHQSA-N
Formula:	C10H8N2OS
SMILES:	<chem>N=C1NC(=O)C(=Cc2ccccc2)S1</chem>
Mol. weight [g/mol]:	204.25
CAS:	14230-00-3

Physical Properties

Property code	Value	Unit	Source
gf	417.82	kJ/mol	Joback Method
hf	255.95	kJ/mol	Joback Method
hvap	71.13	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	1.825		Crippen Method
mvol	146.420	ml/mol	McGowan Method
tb	732.61	K	Joback Method
tf	609.26	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.52	J/molxK	732.61	Joback Method
cpg	59.11	J/molxK	100.12	Joback Method
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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=C14230003&Units=SI

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
log₁₀w_s:	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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