4,4,6-Trimethyl-2-phenylimino-4H-1,3-thiazine

Inchi: InChI=1S/C13H16N2S/c1-10-9-13(2,3)15-12(16-10)14-11-7-5-4-6-8-11/h4-9H,1-3H3,(H,1
InchiKey: NIESPHSLDFVWAU-UHFFFAOYSA-N
Formula: C13H16N2S
SMILES: CC1=CC(C)(C)NC(=Nc2ccccc2)S1
Mol. weight [g/mol]: 232.34
CAS: 27058-61-3

Physical Properties

Property code	Value	Unit	Source
hf	164.85	kJ/mol	Joback Method
hvap	63.75	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.693		Crippen Method
mcvol	187.120	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
tb	722.99	K	Joback Method
tc	997.65	K	Joback Method

Sources

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=C27058613&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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