2-Methyl-1,3-diphenyl-2-thiopseudourea

Inchi: InChI=1S/C14H14N2S/c1-17-14(15-12-8-4-2-5-9-12)16-13-10-6-3-7-11-13/h2-11H,1H3,(
InchiKey: KZXMKHQCJVVAQG-UHFFFAOYSA-N
Formula: C14H14N2S
SMILES: CSC(=Nc1ccccc1)Nc1ccccc1
Mol. weight [g/mol]: 242.34
CAS: 5416-30-8

Physical Properties

Property code	Value	Unit	Source
hf	308.54	kJ/mol	Joback Method
hvap	67.96	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	4.149		Crippen Method
mcvol	192.610	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
tb	768.59	K	Joback Method
tc	1040.25	K	Joback Method

Sources

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=C5416308&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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