1,5-DIPHENYL-3-THIOCARBOHYDRAZIDE

Inchi: InChI=1S/C13H14N4S/c18-13(16-14-11-7-3-1-4-8-11)17-15-12-9-5-2-6-10-12/h1-10,14-1
InchiKey: BNSNUHPJRKTRNT-UHFFFAOYSA-N
Formula: C13H14N4S
SMILES: S=C(NNc1ccccc1)NNc1ccccc1
Mol. weight [g/mol]: 258.35

Physical Properties

Property code	Value	Unit	Source
hf	368.29	kJ/mol	Cheméo Relay (1.0)
hfus	42.51	kJ/mol	Joback Method
hvap	135.13	kJ/mol	Cheméo Relay (1.0)
ie	7.36	eV	Cheméo Relay (1.0)
log10ws	-4.27		Cheméo Relay (1.0)
logp	2.505		Crippen Method
mcvol	198.480	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
tb	644.06	K	Cheméo Relay (1.0)
tc	1035.78	K	Cheméo Relay (1.0)
tf	451.75	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.30	J/mol×K	820.92	Joback Method
cpg	562.30	J/mol×K	863.24	Joback Method
cpg	573.36	J/mol×K	905.56	Joback Method
cpg	583.62	J/mol×K	947.87	Joback Method
cpg	593.26	J/mol×K	990.19	Joback Method
cpg	602.42	J/mol×K	1032.51	Joback Method
cpg	611.26	J/mol×K	1074.83	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C622037&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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