1,4-Diphenylsemicarbazide

Other names:	Hydrazinecarboxamide, N,2-diphenyl- N,N'-Diphenyl semicarbazide Semicarbazide, 1,4-diphenyl- 1,4-Diphenylsemicarbizide
Inchi:	InChI=1S/C13H13N3O/c17-13(14-11-7-3-1-4-8-11)16-15-12-9-5-2-6-10-12/h1-10,15H,(H
InchiKey:	NGZZNUMYERKSQA-UHFFFAOYSA-N
Formula:	C13H13N3O
SMILES:	O=C(NNc1ccccc1)Nc1ccccc1
Mol. weight [g/mol]:	227.26
CAS:	621-12-5

Physical Properties

Property code	Value	Unit	Source
gf	422.65	kJ/mol	Joback Method
hf	209.24	kJ/mol	Joback Method
hfus	34.40	kJ/mol	Joback Method
hvap	75.14	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.835		Crippen Method
mcvol	178.020	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
tb	754.58	K	Joback Method
tc	997.35	K	Joback Method
tf	497.02	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.26	J/mol×K	754.58	Joback Method
cpg	503.19	J/mol×K	795.04	Joback Method
cpg	514.97	J/mol×K	835.50	Joback Method
cpg	525.67	J/mol×K	875.96	Joback Method
cpg	535.37	J/mol×K	916.43	Joback Method

cpg	544.17	J/mol×K	956.89	Joback Method
cpg	552.15	J/mol×K	997.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C621125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume