

N-isopropylidene-N'-phenylhydrazine

Other names:	Acetone phenylhydrazone N-Isopropylidene-N'-phenylhydrazine
Inchi:	InChI=1S/C9H12N2/c1-8(2)10-11-9-6-4-3-5-7-9/h3-7,11H,1-2H3
InchiKey:	JQLKSEQEILIJEG-UHFFFAOYSA-N
Formula:	C9H12N2
SMILES:	CC(C)=NNc1ccccc1
Mol. weight [g/mol]:	148.21

Physical Properties

Property code	Value	Unit	Source
af	0.4938		Cheméo Relay (1.0)
chl	-5095.30	kJ/mol	NIST Webbook
gf	290.71	kJ/mol	Cheméo Relay (1.0, beta)
hf	189.37	kJ/mol	Cheméo Relay (1.0)
hfl	-161.30	kJ/mol	NIST Webbook
hfs	-192.00	kJ/mol	NIST Webbook
hvap	64.84	kJ/mol	Cheméo Relay (1.0)
ie	7.68	eV	Cheméo Relay (1.0)
log10ws	-1.48		Cheméo Relay (1.0)
logp	2.494		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	521.11	K	Cheméo Relay (1.0)
tc	754.54	K	Cheméo Relay (1.0)
tf	319.02	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	74.60	kJ/mol	424.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	436.20	K	6.70	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C103026&Units=SI>

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

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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