

Phenicarbazide

Other names:	Hydrazinecarboxamide, 2-phenyl- Semicarbazide, 1-phenyl- Carbaphen Cryogenine Cryogenine (pharmaceutical) Febrimin Phenicarbazid Phenygenine Phenylsemicarbazide 1-Carbamoyl-2-phenylhydrazine 1-Carbamyl-2-phenylhydrazine 1-Phenylsemicarbazide Carbamic acid, 2-phenylhydrazide Hydrazine, 1-carbamoyl-2-phenyl- Kryogenin 1-Phenylhydrazinecarboxamide 2-Phenylhydrazide carbamic acid 2-Phenylhydrazinecarboxamide Fenylsemikarbazid NSC 2763
Inchi:	InChI=1S/C7H9N3O/c8-7(11)10-9-6-4-2-1-3-5-6/h1-5,9H,(H3,8,10,11)
InchiKey:	AVKHCKXGKPAGEI-UHFFFAOYSA-N
Formula:	C7H9N3O
SMILES:	NC(=O)NNc1ccccc1
Mol. weight [g/mol]:	151.17
CAS:	103-03-7

Physical Properties

Property code	Value	Unit	Source
gf	236.78	kJ/mol	Joback Method
hf	76.87	kJ/mol	Joback Method
hfus	24.92	kJ/mol	Joback Method
hvap	63.71	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	0.682		Crippen Method
mvol	117.240	ml/mol	McGowan Method
pc	5008.59	kPa	Joback Method

tb	612.98	K	Joback Method
tc	847.56	K	Joback Method
tf	433.58	K	Joback Method
vc	0.424	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.95	J/mol×K	612.98	Joback Method
cpg	296.72	J/mol×K	652.08	Joback Method
cpg	306.66	J/mol×K	691.17	Joback Method
cpg	315.80	J/mol×K	730.27	Joback Method
cpg	324.19	J/mol×K	769.36	Joback Method
cpg	331.88	J/mol×K	808.46	Joback Method
cpg	338.89	J/mol×K	847.56	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=C103037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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