

Semicarbazide, 4-methyl-

Inchi:	InChI=1S/C2H7N3O/c1-4-2(6)5-3/h3H2,1H3,(H2,4,5,6)
InchiKey:	LHYKTQVFLKHQSR-UHFFFAOYSA-N
Formula:	C2H7N3O
SMILES:	CNC(=O)NN
Mol. weight [g/mol]:	89.10
CAS:	17696-95-6

Physical Properties

Property code	Value	Unit	Source
gf	82.27	kJ/mol	Joback Method
hf	-56.46	kJ/mol	Joback Method
hfus	17.93	kJ/mol	Joback Method
hvap	50.30	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	-1.211		Crippen Method
mcvol	70.550	ml/mol	McGowan Method
pc	6259.01	kPa	Joback Method
tb	471.90	K	Joback Method
tc	677.70	K	Joback Method
tf	350.81	K	Joback Method
vc	0.253	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.54	J/molxK	471.90	Joback Method
cpg	156.51	J/molxK	506.20	Joback Method
cpg	163.13	J/molxK	540.50	Joback Method
cpg	169.39	J/molxK	574.80	Joback Method
cpg	175.31	J/molxK	609.10	Joback Method
cpg	180.89	J/molxK	643.40	Joback Method
cpg	186.15	J/molxK	677.70	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=C17696956&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

Latest version available from:

<https://www.chemeo.com/cid/12-802-7/Semicarbazide-4-methyl.pdf>

Generated by Cheméo on 2025-03-21 17:13:21.960107033 +0000 UTC m=+5785417.807032661.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.