SEMICARBAZIDE

Other names:	Semicarbazide
	Aminomocovina
	Aminourea
	Carbamic acid, hydrazide
	Carbamylhydrazine
	Carbazamide
	Hydrazine, carbamoyl-
	Semikarbazid
	Urea, amino-
Inchi:	InChI=1S/CH5N3O/c2-1(5)4-3/h3H2,(H3,2,4,5)
InchiKey:	DUIOPKIIICUYRZ-UHFFFAOYSA-N
Formula:	CH5N3O
SMILES:	NNC(N)=O
Mol. weight [g/mol]:	75.07

Physical Properties

Property code	Value	Unit	Source
chs	-882.40 ± 0.66	kJ/mol	NIST Webbook
hf	-139.15	kJ/mol	Cheméo Relay (1.0)
hfs	-225.68 ± 0.60	kJ/mol	NIST Webbook
hfus	15.44	kJ/mol	Joback Method
hvap	64.08	kJ/mol	Cheméo Relay (1.0)
ie	9.38	eV	Cheméo Relay (1.0)
log10ws	0.18		Cheméo Relay (1.0)
logp	-1.472		Crippen Method
mcvol	56.460	ml/mol	McGowan Method
ss	119.60	J/mol×K	NIST Webbook
ss	119.60	J/mol×K	NIST Webbook
tb	511.32	K	Cheméo Relay (1.0)
tf	416.87	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	118.56	J/mol×K	471.38	Joback Method
cpg	123.82	J/mol×K	507.92	Joback Method
cpg	128.78	J/mol×K	544.46	Joback Method
cpg	133.46	J/mol×K	580.99	Joback Method
cpg	137.86	J/mol×K	617.53	Joback Method
cpg	141.98	J/mol×K	654.07	Joback Method
cpg	145.83	J/mol×K	690.61	Joback Method
cps	110.60	J/mol×K	298.15	NIST Webbook
cps	110.60	J/mol×K	298.15	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57567&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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
ss: Solid phase molar entropy at standard conditions
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point