

CONIINE

Other names:	(+)-Coniine
	(S)-(+)-Coniine
	(S)-2-Propylpiperidine
	(S)-Coniine
	2-Propylpiperidine
	Cicutin
	Cicutine
	Conicine
	Coniin
	Koniin
	Piperidine, 2-propyl-, (2S)-
	d-Conicine
Inchi:	InChI=1S/C8H17N/c1-2-5-8-6-3-4-7-9-8/h8-9H,2-7H2,1H3
InchiKey:	NDNUANOUGZGEPO-UHFFFAOYSA-N
Formula:	C8H17N
SMILES:	CCCC1CCCCN1
Mol. weight [g/mol]:	127.23

Physical Properties

Property code	Value	Unit	Source
af	0.3578		Cheméo Relay (1.0)
gf	128.64	kJ/mol	Joback Method
hf	-109.08	kJ/mol	Cheméo Relay (1.0)
hfus	17.90	kJ/mol	Joback Method
hvap	47.82	kJ/mol	Cheméo Relay (1.0)
ie	8.12	eV	Cheméo Relay (1.0)
log10ws	-1.50		Aqueous Solubility Prediction Method
logp	1.929		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	992.00		NIST Webbook
rinpol	992.00		NIST Webbook
tb	443.56	K	Cheméo Relay (1.0)
tc	644.10	K	Cheméo Relay (1.0)
tf	239.89	K	Cheméo Relay (1.0)
vc	0.436	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.94	J/mol×K	450.54	Joback Method
cpg	275.63	J/mol×K	485.34	Joback Method
cpg	292.49	J/mol×K	520.15	Joback Method
cpg	308.53	J/mol×K	554.95	Joback Method
cpg	323.77	J/mol×K	589.76	Joback Method
cpg	338.23	J/mol×K	624.56	Joback Method
cpg	351.91	J/mol×K	659.37	Joback Method

Sources

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C458888&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>

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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