Cyclopentene, 1-cyanomethyl-

Other names:	1-Cyclopentenylacetonitrile
	(1-Cyclopenten-1-yl)-acetonitrile
	1-Cyclopentene-1-acetonitrile
	cyclopent-1-ene-1-acetonitrile
Inchi:	InChI=1S/C7H9N/c8-6-5-7-3-1-2-4-7/h3H,1-2,4-5H2
InchiKey:	LEWVRAMNXUWSFL-UHFFFAOYSA-N
Formula:	C7H9N
SMILES:	N#CCC1=CCCC1
Mol. weight [g/mol]:	107.16

Physical Properties

Property code	Value	Unit	Source
hf	157.82	kJ/mol	Cheméo Relay (1.0)
hfus	9.09	kJ/mol	Joback Method
hvap	55.28	kJ/mol	Cheméo Relay (1.0)
ie	9.38	eV	Cheméo Relay (1.0)
logp	2.010		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
tb	470.85	K	Cheméo Relay (1.0)
tf	226.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.81	J/mol×K	485.73	Joback Method
cpg	205.91	J/mol×K	522.76	Joback Method
cpg	216.32	J/mol×K	559.80	Joback Method
cpg	226.07	J/mol×K	596.83	Joback Method
cpg	235.19	J/mol×K	633.87	Joback Method
cpg	243.73	J/mol×K	670.90	Joback Method
cpg	251.72	J/mol×K	707.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	397.20	K	13.30	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22734049&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point