

1-Cyclopentylacetonitrile

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]:	107.15
CAS:	22734-04-9

Physical Properties

Property code	Value	Unit	Source
gf	205.83	kJ/mol	Joback Method
hf	104.20	kJ/mol	Joback Method
hfus	9.09	kJ/mol	Joback Method
hvap	43.17	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.010		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	485.73	K	Joback Method
tc	707.93	K	Joback Method
tf	262.06	K	Joback Method
vc	0.382	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.81	J/molxK	485.73	Joback Method
cpg	205.91	J/molxK	522.76	Joback Method
cpg	216.32	J/molxK	559.80	Joback Method
cpg	226.07	J/molxK	596.83	Joback Method
cpg	235.19	J/molxK	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22734049&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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