

4-Cyanocyclohexene

Other names:	3-Cyclohexene-1-carbonitrile 3-Cyclohexenecarbonitrile Tetrahydrobenzonitrile 4-Cyanocyclohexene-1 4-Cyano-1-cyclohexene 1-Cyano-3-cyclohexene 3-Cyclohexenyl cyanide 3-Cyklohexenylkyanid 4-Cyclohexenecarbonitrile
Inchi:	InChI=1S/C7H9N/c8-6-7-4-2-1-3-5-7/h1-2,7H,3-5H2
InchiKey:	GYBNBQFUPDFFQX-UHFFFAOYSA-N
Formula:	C7H9N
SMILES:	N#CC1CC=CCC1
Mol. weight [g/mol]:	107.15
CAS:	100-45-8

Physical Properties

Property code	Value	Unit	Source
gf	195.65	kJ/mol	Joback Method
hf	89.17	kJ/mol	Joback Method
hfus	8.45	kJ/mol	Joback Method
hvap	42.38	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.866		Crippen Method
mcvol	95.710	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	480.35	K	Joback Method
tc	709.84	K	Joback Method
tf	241.78	K	Joback Method
vc	0.372	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	195.24	J/mol×K	480.35	Joback Method
cpg	208.07	J/mol×K	518.60	Joback Method
cpg	220.11	J/mol×K	556.85	Joback Method
cpg	231.38	J/mol×K	595.09	Joback Method
cpg	241.92	J/mol×K	633.34	Joback Method
cpg	251.74	J/mol×K	671.59	Joback Method
cpg	260.88	J/mol×K	709.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.50 ± 0.50	K	3.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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