

Cyclohexane, (nitromethylene)-

Inchi:	InChI=1S/C7H11NO2/c9-8(10)6-7-4-2-1-3-5-7/h6H,1-5H2
InchiKey:	JVQOIOZEAYCROA-UHFFFAOYSA-N
Formula:	C7H11NO2
SMILES:	O=[N+](O-)C=C1CCCCC1
Mol. weight [g/mol]:	141.17
CAS:	27861-39-8

Physical Properties

Property code	Value	Unit	Source
gf	121.23	kJ/mol	Joback Method
hf	-47.88	kJ/mol	Joback Method
hfus	16.33	kJ/mol	Joback Method
hvap	49.29	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.111		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
tb	542.26	K	Joback Method
tc	790.41	K	Joback Method
tf	334.24	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.62	J/molxK	542.26	Joback Method
cpg	273.31	J/molxK	583.62	Joback Method
cpg	286.93	J/molxK	624.98	Joback Method
cpg	299.54	J/molxK	666.33	Joback Method
cpg	311.20	J/molxK	707.69	Joback Method
cpg	321.96	J/molxK	749.05	Joback Method
cpg	331.87	J/molxK	790.41	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27861398&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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