

Cyclohexene, 1-nitro-

Other names:	1-Nitrocyclohexene 1-Nitrocyclohex-1-ene 1-Nitro-1-cyclohexene
Inchi:	InChI=1S/C6H9NO2/c8-7(9)6-4-2-1-3-5-6/h4H,1-3,5H2
InchiKey:	DJBRXNRKYAWTBL-UHFFFAOYSA-N
Formula:	C6H9NO2
SMILES:	O=[N+](O-)C1=CCCCC1
Mol. weight [g/mol]:	127.14
CAS:	2562-37-0

Physical Properties

Property code	Value	Unit	Source
gf	87.68	kJ/mol	Joback Method
hf	-56.96	kJ/mol	Joback Method
hfus	14.25	kJ/mol	Joback Method
hvap	47.23	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.721		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
ripol	1174.00		NIST Webbook
ripol	1174.00		NIST Webbook
ripol	1174.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1784.00		NIST Webbook
tb	516.88	K	Joback Method
tc	765.52	K	Joback Method
tf	325.89	K	Joback Method
vc	0.373	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	215.00	J/mol×K	516.88	Joback Method
cpg	228.26	J/mol×K	558.32	Joback Method
cpg	240.57	J/mol×K	599.76	Joback Method
cpg	251.98	J/mol×K	641.20	Joback Method
cpg	262.53	J/mol×K	682.64	Joback Method
cpg	272.26	J/mol×K	724.08	Joback Method
cpg	281.21	J/mol×K	765.52	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	340.20	K	0.10	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2562370&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
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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