Cyclohexane, nitro-

Other names: Nitrocyclohexane
Inchi: InChI=1S/C6H11NO2/c8-7(9)6-4-2-1-3-5-6/h6H,1-5H2
InchiKey: NJNQUTDUIPVROZ-UHFFFAOYSA-N
Formula: C6H11NO2
SMILES: O=[N+]([O-])C1CCCCC1
Mol. weight [g/mol]: 129.16
CAS: 1122-60-7

Physical Properties

Property code	Value	Unit	Source
gf	59.64	kJ/mol	Joback Method
hf	-123.61	kJ/mol	Joback Method
hfus	14.49	kJ/mol	Joback Method
hvap	54.70 ± 0.60	kJ/mol	NIST Webbook
log10ws	-2.42		Crippen Method
logp	1.596		Crippen Method
mcvol	101.960	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
rinpol	1079.00		NIST Webbook
rinpol	1083.00		NIST Webbook
ripol	1645.00		NIST Webbook
ripol	1645.00		NIST Webbook
tb	508.07	K	Joback Method
tc	752.72	K	Joback Method
tf	308.37	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.86	J/mol×K	508.07	Joback Method
cpg	249.44	J/mol×K	548.85	Joback Method
cpg	263.97	J/mol×K	589.62	Joback Method
cpg	277.50	J/mol×K	630.40	Joback Method

cpg	290.05	J/mol×K	671.17	Joback Method
cpg	301.66	J/mol×K	711.95	Joback Method
cpg	312.38	J/mol×K	752.72	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	478.70	K	102.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1122607&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
rinpol: Non-polar retention indices
ripol: 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