Cyclohexanone, 2-nitro-

Other names: «alpha»-Nitrocyclohexanone
2-Nitrocyclohexanone
Inchi: InChI=1S/C6H9NO3/c8-6-4-2-1-3-5(6)7(9)10/h5H,1-4H2
InchiKey: SZNILIWUUKKNPE-UHFFFAOYSA-N
Formula: C6H9NO3
SMILES: O=C1CCCCC1[N+](=O)[O-]
Mol. weight [g/mol]: 143.14
CAS: 4883-67-4

Physical Properties

Property code	Value	Unit	Source
gf	-62.95	kJ/mol	Joback Method
hf	-261.31	kJ/mol	Joback Method
hfus	14.00	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	0.775		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
tb	575.89	K	Joback Method
tc	836.44	K	Joback Method
tf	376.59	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.04	J/mol×K	575.89	Joback Method
cpg	272.86	J/mol×K	619.32	Joback Method
cpg	286.70	J/mol×K	662.74	Joback Method
cpg	299.54	J/mol×K	706.17	Joback Method
cpg	311.37	J/mol×K	749.59	Joback Method
cpg	322.18	J/mol×K	793.02	Joback Method
cpg	331.95	J/mol×K	836.44	Joback Method

Sources

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=C4883674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume