1-Nitro-2-propanone

Other names: 2-Propanone, 1-nitro-
Nitropropanone
Nitroacetone
Inchi: InChI=1S/C3H5NO3/c1-3(5)2-4(6)7/h2H2,1H3
InchiKey: QCDJOJKIHZQJGX-UHFFFAOYSA-N
Formula: C3H5NO3
SMILES: CC(=O)C[N+](=O)[O-]
Mol. weight [g/mol]: 103.08
CAS: 10230-68-9

Physical Properties

Property code	Value	Unit	Source
chs	-1600.00 ± 0.63	kJ/mol	NIST Webbook
gf	-118.99	kJ/mol	Joback Method
hf	-228.59	kJ/mol	Joback Method
hfs	-295.00 ± 0.63	kJ/mol	NIST Webbook
hfus	16.49	kJ/mol	Joback Method
hvap	45.61	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	-0.148		Crippen Method
mcvol	72.120	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	473.75	K	Joback Method
tc	695.13	K	Joback Method
tf	317.11	K	Joback Method
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.71	J/mol×K	473.75	Joback Method
cpg	149.71	J/mol×K	510.65	Joback Method
cpg	156.32	J/mol×K	547.54	Joback Method
cpg	162.55	J/mol×K	584.44	Joback Method

cpg	168.40	J/mol×K	621.34	Joback Method
cpg	173.88	J/mol×K	658.23	Joback Method
cpg	179.02	J/mol×K	695.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.70	K	3.20	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10230689&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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