Nitroethylene

Inchi: InChI=1S/C2H3NO2/c1-2-3(4)5/h2H,1H2
InchiKey: RPMXALUWKZHYOV-UHFFFAOYSA-N
Formula: C2H3NO2
SMILES: C=C[N+](=O)[O-]
Mol. weight [g/mol]: 73.05
CAS: 3638-64-0

Physical Properties

Property code	Value	Unit	Source
ea	1.65	eV	NIST Webbook
gf	89.35	kJ/mol	Joback Method
hf	30.06	kJ/mol	Joback Method
hfus	11.02	kJ/mol	Joback Method
hvap	35.97	kJ/mol	Joback Method
ie	10.85	eV	NIST Webbook
ie	11.00	eV	NIST Webbook
log10ws	-1.09		Crippen Method
logp	0.407		Crippen Method
mcvol	52.160	ml/mol	McGowan Method
pc	5438.52	kPa	Joback Method
tb	371.70	K	NIST Webbook
tc	610.44	K	Joback Method
tf	254.15	K	Joback Method
vc	0.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	85.27	J/mol×K	393.68	Joback Method
cpg	90.51	J/mol×K	429.81	Joback Method
cpg	95.44	J/mol×K	465.93	Joback Method
cpg	100.06	J/mol×K	502.06	Joback Method
cpg	104.38	J/mol×K	538.19	Joback Method
cpg	108.43	J/mol×K	574.31	Joback Method

cpg	112.22	J/mol×K	610.44	Joback Method

Sources

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=C3638640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
ie:	Ionization energy
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