Ethanamine, N-ethyl-N-nitro-

Other names: Diethylamine, N-nitro-
Diethylnitramine
N-Nitrodiethylamine
Inchi: InChI=1S/C4H10N2O2/c1-3-5(4-2)6(7)8/h3-4H2,1-2H3
InchiKey: QAXAHXNXXIWQIZ-UHFFFAOYSA-N
Formula: C4H10N2O2
SMILES: CCN(CC)[N+](=O)[O-]
Mol. weight [g/mol]: 118.13
CAS: 7119-92-8

Physical Properties

Property code	Value	Unit	Source
chl	-2897.00 ± 8.40	kJ/mol	NIST Webbook
chl	-2896.00	kJ/mol	NIST Webbook
gf	129.13	kJ/mol	Joback Method
hf	-69.12	kJ/mol	Joback Method
hfl	-106.00 ± 8.40	kJ/mol	NIST Webbook
hfus	20.50	kJ/mol	Joback Method
hvap	43.13	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	0.520		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	3945.61	kPa	Joback Method
tb	455.20	K	Joback Method
tc	659.57	K	Joback Method
tf	310.92	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.50	J/mol×K	455.20	Joback Method
cpg	209.93	J/mol×K	489.26	Joback Method
cpg	219.79	J/mol×K	523.32	Joback Method

cpg	229.10	J/mol×K	557.39	Joback Method
cpg	237.88	J/mol×K	591.45	Joback Method
cpg	246.15	J/mol×K	625.51	Joback Method
cpg	253.93	J/mol×K	659.57	Joback Method
hvapt	49.70	kJ/mol	358.00	NIST Webbook
hvapt	53.10 ± 3.30	kJ/mol	338.00	NIST Webbook

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=C7119928&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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