N-ethyl-4-nitroaniline

Other names: N-ethyl-4-nitrobenzenamine
Inchi: InChI=1S/C8H10N2O2/c1-2-9-7-3-5-8(6-4-7)10(11)12/h3-6,9H,2H2,1H3
InchiKey: XBNNLAWQCMDISJ-UHFFFAOYSA-N
Formula: C8H10N2O2
SMILES: CCNc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 166.18

Physical Properties

Property code	Value	Unit	Source
gf	244.20	kJ/mol	Joback Method
hf	59.32	kJ/mol	Joback Method
hfus	22.70	kJ/mol	DSC measurement and prediction of phase diagrams for binary mixtures of energetic materials' stabilizers
hvap	59.37	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.027		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
tb	616.11	K	Joback Method
tc	858.52	K	Joback Method
tf	368.21	K	DSC measurement and prediction of phase diagrams for binary mixtures of energetic materials' stabilizers
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.89	J/mol×K	616.11	Joback Method
cpg	322.05	J/mol×K	656.51	Joback Method
cpg	333.31	J/mol×K	696.91	Joback Method
cpg	343.71	J/mol×K	737.31	Joback Method

cpg	353.30	J/mol×K	777.71	Joback Method
cpg	362.13	J/mol×K	818.12	Joback Method
cpg	370.24	J/mol×K	858.52	Joback Method

Sources

DSC measurement and prediction of phase diagrams for binary mixtures of energetic materials' stabilizers:	https://www.doi.org/10.1016/j.tca.2013.04.021
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
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