1-Ethyl-3-nitrobenzene

Other names: Benzene, 1-ethyl-3-nitro-
Nitrobenzene, 3-ethyl-
Inchi: InChI=1S/C8H9NO2/c1-2-7-4-3-5-8(6-7)9(10)11/h3-6H,2H2,1H3
InchiKey: RXAKLPGKSXJZEF-UHFFFAOYSA-N
Formula: C8H9NO2
SMILES: CCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 151.16
CAS: 7369-50-8

Physical Properties

Property code	Value	Unit	Source
gf	154.81	kJ/mol	Joback Method
hf	5.85	kJ/mol	Joback Method
hfus	21.49	kJ/mol	Joback Method
hvap	52.93	kJ/mol	Joback Method
ie	9.64 ± 0.03	eV	NIST Webbook
log10ws	-2.93		Crippen Method
logp	2.157		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
tb	514.15 ± 2.00	K	NIST Webbook
tb	515.70	K	NIST Webbook
tc	810.58	K	Joback Method
tf	362.47	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.21	J/mol×K	565.94	Joback Method
cpg	277.45	J/mol×K	606.71	Joback Method
cpg	288.81	J/mol×K	647.49	Joback Method
cpg	299.33	J/mol×K	688.26	Joback Method
cpg	309.07	J/mol×K	729.03	Joback Method

cpg	318.05	J/mol×K	769.80	Joback Method
cpg	326.32	J/mol×K	810.58	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49708e+01
Coeff. B	-4.46398e+03
Coeff. C	-8.45010e+01
Temperature range (K), min.	388.52
Temperature range (K), max.	546.64

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7369508&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pc: Critical Pressure

pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume