Benzene, 1-ethyl-2-nitro-

Other names:	1-Ethyl-2-nitrobenzene
	2-ETHYL-1-NITROBENZENE
	2-Ethylnitrobenzene
	O-ETHYLNITROBENZENE
	O-NITROETHYLBENZENE
Inchi:	InChI=1S/C8H9NO2/c1-2-7-5-3-4-6-8(7)9(10)11/h3-6H,2H2,1H3
InchiKey:	PXWYZLWEKCMTEZ-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	CCc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	151.16
CAS:	612-22-6

Physical Properties

Property code	Value	Unit	Source
chl	-4385.67	kJ/mol	NIST Webbook
gf	154.81	kJ/mol	Joback Method
hf	5.85	kJ/mol	Joback Method
hfl	-48.66	kJ/mol	NIST Webbook
hfus	21.49	kJ/mol	Joback Method
hvap	63.00 ± 0.40	kJ/mol	NIST Webbook
ie	9.39 ± 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
ripol	1910.00		NIST Webbook
ripol	1910.00		NIST Webbook
tb	565.94	K	Joback Method
tc	810.58	K	Joback Method
tf	260.90 ± 0.02	K	NIST Webbook
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
hvapt	62.70 ± 0.40	kJ/mol	303.50	NIST Webbook
hvapt	56.30	kJ/mol	387.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41475e+01
Coeff. B	-4.14134e+03
Coeff. C	-8.17210e+01
Temperature range (K), min.	380.52
Temperature range (K), max.	550.41

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.00875e+01
Coeff. B	-9.62909e+03
Coeff. C	-9.26164e+00
Coeff. D	5.44991e-06
Temperature range (K), min.	353.15
Temperature range (K), max.	433.15

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1454
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1454
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C612226&Units=SI

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume