

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]:	151.17
CAS:	7369-50-8

Physical Properties

Property code	Value	Unit	Source
af	0.4992		Cheméo Relay (1.0)
gf	154.81	kJ/mol	Joback Method
hf	12.35	kJ/mol	Cheméo Relay (1.0)
hfus	21.49	kJ/mol	Joback Method
hvap	63.86	kJ/mol	Cheméo Relay (1.0)
ie	9.64 ± 0.03	eV	NIST Webbook
log10ws	-3.02		Cheméo Relay (1.0)
logp	2.157		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
tb	515.70	K	NIST Webbook
tb	514.15 ± 2.00	K	NIST Webbook
tc	748.44	K	Cheméo Relay (1.0)
tf	256.96	K	Cheméo Relay (1.0)
vc	0.412	m3/kmol	Cheméo Relay (1.0)

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	$\ln(P_{vp}) = A + B/(T + C)$
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

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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

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

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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

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