

Benzene, 1-ethyl-4-nitro-

Other names:	1-Ethyl-4-nitrobenzene 4-Ethylnitrobenzene 4-Nitroethylbenzene p-Ethylnitrobenzene p-Nitroethylbenzene p-Nitrophenylethane
Inchi:	InChI=1S/C8H9NO2/c1-2-7-3-5-8(6-4-7)9(10)11/h3-6H,2H2,1H3
InchiKey:	RESTWAHJFMZUIZ-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	CCc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	151.16
CAS:	100-12-9

Physical Properties

Property code	Value	Unit	Source
chs	-4379.02	kJ/mol	NIST Webbook
gf	154.81	kJ/mol	Joback Method
hf	5.85	kJ/mol	Joback Method
hfs	-55.31	kJ/mol	NIST Webbook
hfus	21.49	kJ/mol	Joback Method
hvap	52.93	kJ/mol	Joback Method
ie	9.71 ± 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	2057.00		NIST Webbook
ripol	2057.00		NIST Webbook
tb	518.70	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
hvapt	59.40	kJ/mol	393.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64817e+01
Coeff. B	-5.67106e+03
Coeff. C	-4.06670e+01
Temperature range (K), min.	390.86
Temperature range (K), max.	548.36

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C100129&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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid 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

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