Benzene, 1-ethoxy-3-nitro-

Other names:	Phenetole, m-nitro-
	m-Nitrophenetole
	1-Ethoxy-3-nitrobenzene
	3-Nitrophenetole
Inchi:	InChI=1S/C8H9NO3/c1-2-12-8-5-3-4-7(6-8)9(10)11/h3-6H,2H2,1H3
InchiKey:	LFOLBPDHVGDKGJ-UHFFFAOYSA-N
Formula:	C8H9NO3
SMILES:	CCOc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	167.16
CAS:	621-52-3

Physical Properties

Property code	Value	Unit	Source
gf	49.81	kJ/mol	Joback Method
hf	-126.37	kJ/mol	Joback Method
hfus	22.68	kJ/mol	Joback Method
hvap	55.34	kJ/mol	Joback Method
ie	9.11 ± 0.15	eV	NIST Webbook
log10ws	-2.66		Crippen Method
logp	1.994		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
tb	588.36	K	Joback Method
tc	829.28	K	Joback Method
tf	384.70	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.63	J/mol×K	588.36	Joback Method
cpg	299.65	J/mol×K	628.51	Joback Method
cpg	310.86	J/mol×K	668.67	Joback Method
cpg	321.29	J/mol×K	708.82	Joback Method

cpg	330.96	J/mol×K	748.97	Joback Method
cpg	339.88	J/mol×K	789.13	Joback Method
cpg	348.07	J/mol×K	829.28	Joback Method

Sources

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=C621523&Units=SI
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
ie:	Ionization energy
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