Ethane, nitro-

Other names:	C2H5NO2
	NE
	Nitroetan
	Nitroethane
	Nitroparaffin
	UN 2842
Inchi:	InChI=1S/C2H5NO2/c1-2-3(4)5/h2H2,1H3
InchiKey:	MCSAJNNLRCFZED-UHFFFAOYSA-N
Formula:	C2H5NO2
SMILES:	CC[N+](=O)[O-]
Mol. weight [g/mol]:	75.07
CAS:	79-24-3

Physical Properties

Property code	Value	Unit	Source
af	0.3410		KDB
affp	765.70	kJ/mol	NIST Webbook
basg	733.20	kJ/mol	NIST Webbook
chl	-1358.00 ± 1.00	kJ/mol	NIST Webbook
chl	-1361.60 ± 1.30	kJ/mol	NIST Webbook
chl	-1358.00 ± 0.40	kJ/mol	NIST Webbook
gf	1.51	kJ/mol	Joback Method
hf	-95.37	kJ/mol	Joback Method
hfl	-143.60 ± 1.10	kJ/mol	NIST Webbook
hfl	-140.10 ± 1.30	kJ/mol	NIST Webbook
hfl	-144.00 ± 0.40	kJ/mol	NIST Webbook
hfus	12.30	kJ/mol	Joback Method
hvap	41.60 ± 0.42	kJ/mol	NIST Webbook
ie	10.92 ± 0.01	eV	NIST Webbook
ie	11.02	eV	NIST Webbook
ie	10.88 ± 0.05	eV	NIST Webbook
ie	10.90 ± 0.05	eV	NIST Webbook
log10ws	-0.22		Aqueous Solubility Prediction Method
log10ws	-0.22		Estimated Solubility Method
logp	0.283		Crippen Method

mcvol	56.460	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=1)		KDB
nfpas	%!d(float64=2)		KDB
pc	4850.00	kPa	KDB
rinpol	636.89		NIST Webbook
rinpol	590.00		NIST Webbook
rinpol	583.00		NIST Webbook
rinpol	598.00		NIST Webbook
rinpol	590.00		NIST Webbook
rinpol	618.00		NIST Webbook
rinpol	623.00		NIST Webbook
rinpol	618.00		NIST Webbook
rinpol	655.00		NIST Webbook
rinpol	590.00		NIST Webbook
rinpol	618.58		NIST Webbook
rinpol	615.90		NIST Webbook
rinpol	617.81		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	592.00		NIST Webbook
rinpol	623.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	638.00		NIST Webbook
rinpol	572.00		NIST Webbook
rinpol	567.80		NIST Webbook
rinpol	617.81		NIST Webbook
rinpol	617.22		NIST Webbook
rinpol	616.67		NIST Webbook
rinpol	616.25		NIST Webbook
rinpol	616.07		NIST Webbook
rinpol	615.90		NIST Webbook
rinpol	616.27		NIST Webbook
rinpol	620.51		NIST Webbook
rinpol	618.58		NIST Webbook
rinpol	619.51		NIST Webbook
rinpol	615.97		NIST Webbook
ripol	1161.00		NIST Webbook
ripol	1196.20		NIST Webbook
ripol	1199.20		NIST Webbook
ripol	1194.20		NIST Webbook
ripol	1181.30		NIST Webbook
ripol	1183.90		NIST Webbook

ripol	1187.30		NIST Webbook
ripol	1190.20		NIST Webbook
ripol	1168.00		NIST Webbook
ripol	1161.00		NIST Webbook
ripol	1179.40		NIST Webbook
tb	387.65 ± 2.00	K	NIST Webbook
tb	387.20	K	KDB
tb	387.40 ± 0.60	K	NIST Webbook
tb	387.22 ± 0.05	K	NIST Webbook
tb	387.90 ± 0.25	K	NIST Webbook
tb	388.20	K	NIST Webbook
tb	387.00 ± 0.60	K	NIST Webbook
tc	595.00	K	KDB
tf	223.00	K	KDB
tf	183.63 ± 0.05	K	NIST Webbook
tf	183.90	K	Aqueous Solubility Prediction Method
tt	183.69 ± 0.04	K	NIST Webbook
vc	0.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.79	J/mol×K	608.77	Joback Method
cpg	127.07	J/mol×K	573.48	Joback Method
cpg	122.07	J/mol×K	538.18	Joback Method
cpg	116.79	J/mol×K	502.89	Joback Method
cpg	111.24	J/mol×K	467.59	Joback Method
cpg	105.38	J/mol×K	432.30	Joback Method
cpg	99.23	J/mol×K	397.00	Joback Method
cpl	134.22	J/mol×K	298.15	NIST Webbook
hfust	9.85	kJ/mol	183.70	NIST Webbook
hfust	9.85	kJ/mol	183.70	NIST Webbook
hfust	9.85	kJ/mol	183.69	NIST Webbook
hvapt	38.60	kJ/mol	356.00	NIST Webbook
hvapt	35.15	kJ/mol	387.20	KDB
hvapt	41.30	kJ/mol	319.50	NIST Webbook

pvap	33.11	kPa	353.15	Vapor-Liquid Equilibria on Four Binary Systems: 2-Phenylpropionaldehyde + Phenol, Propylene Glycol Monomethyl Ether + Nitroethane, Dimethyl Ether + Propylene, and N-Butyric Acid + Propionic Acid
pvap	6.10	kPa	313.15	Vapor-Liquid Equilibria on Four Binary Systems: 2-Phenylpropionaldehyde + Phenol, Propylene Glycol Monomethyl Ether + Nitroethane, Dimethyl Ether + Propylene, and N-Butyric Acid + Propionic Acid
rfi	1.38951		298.15	Isothermal vapor liquid equilibria and excess Gibbs free energies in some binary nitroalkane + chloroalkane mixtures at temperatures from 298.15 K to 318.15 K
rfi	1.38980		298.15	Isothermal Vapor Liquid Equilibria for Nitromethane and Nitroethane + 1,3-Dichloropropane Binary Systems at Temperatures between (343.15 and 363.15) K
rfi	1.38950		298.15	Isothermal (vapour + liquid) equilibria for (nitromethane or nitroethane + 1,4-dichlorobutane) binary systems at temperatures between (343.15 and 363.15) K
sfust	53.64	J/mol×K	183.69	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52739e+01
Coeff. B	-3.77809e+03
Coeff. C	-3.30350e+01
Temperature range (K), min.	285.14
Temperature range (K), max.	412.27

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.04445e+01
Coeff. B	-6.61641e+03
Coeff. C	-6.59835e+00
Coeff. D	3.87418e-06
Temperature range (K), min.	183.63
Temperature range (K), max.	593.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1425
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79243&Units=SI
Isothermal vapour liquid equilibria for 1,2-dichloroethane + nitromethane and 1,2-dichloroethane + nitroethane binary systems at temperatures between 333.15 and 353.15K.:	https://www.doi.org/10.1016/j.fluid.2010.01.024
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1425
Isothermal Vapor Liquid Equilibria for Nitromethane and Nitroethane + 1,3-(nitromethane,nitroethane) + (nitroethane and 1-chlorobutane) ternary systems at temperatures between (343.15 and 368.15) K.:	https://www.doi.org/10.1021/je200651r
Isothermal (vapour + liquid) equilibria for (nitromethane,nitroethane) + (nitroethane and 1-chlorobutane) binary systems at temperatures between (343.15 and 368.15) K.:	https://www.doi.org/10.1016/j.jct.2012.06.033
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1425
Vapor-Liquid Equilibria on Four Binary Systems: 2-Phenylpropionaldehyde + Phenol, Propylene Glycol Monomethyl Ether + Nitroethane, Dimethyl Ether + Propylene, and N-Butyric Acid + Propionic Acid at 101.3 kPa.:	https://www.doi.org/10.1021/je050327l
Isothermal vapor-liquid equilibria and excess Gibbs free energies in some 1-alkanol + 1-chlorobutane mixtures at temperatures from 298.15 K to 318.15 K.:	https://www.doi.org/10.1016/j.fluid.2012.10.015
Estimated Solubility Methodology:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Chapman Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume