Formamide, N,N-diethyl-

Other names:	Diethylamid kyseliny mravenci
	Diethylformamide
	N,N-Diethylformamide
	N-Formyldiethylamine
Inchi:	InChI=1S/C5H11NO/c1-3-6(4-2)5-7/h5H,3-4H2,1-2H3
InchiKey:	SUAKHGWARZSWIH-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CCN(C=O)CC
Mol. weight [g/mol]:	101.15
CAS:	617-84-5

Physical Properties

Property code	Value	Unit	Source
gf	2.48	kJ/mol	Joback Method
hf	-164.58	kJ/mol	Joback Method
hfus	14.02	kJ/mol	Joback Method
hvap	50.30	kJ/mol	NIST Webbook
ie	8.89 ± 0.02	eV	NIST Webbook
log10ws	-0.26		Crippen Method
logp	0.485		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	930.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	895.00		NIST Webbook
ripol	1413.00		NIST Webbook
ripol	1413.00		NIST Webbook
tb	450.70	K	NIST Webbook
tc	546.52	K	Joback Method
tf	220.58	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.86	J/mol×K	403.50	Joback Method
cpg	222.50	J/mol×K	546.52	Joback Method
cpg	214.73	J/mol×K	517.91	Joback Method
cpg	206.59	J/mol×K	489.31	Joback Method
cpg	198.07	J/mol×K	460.71	Joback Method
cpg	189.17	J/mol×K	432.11	Joback Method
cpg	170.14	J/mol×K	374.90	Joback Method
hvapt	48.90	kJ/mol	333.00	NIST Webbook
pvap	1.73	kPa	338.50	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.63	kPa	320.80	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.71	kPa	323.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.85	kPa	325.80	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	1.09	kPa	330.90	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	1.48	kPa	335.90	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.46	kPa	315.70	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	1.95	kPa	340.90	Vapour pressures and enthalpies of vaporisation of alkyl formamides

pvap	2.46	kPa	346.00	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	2.89	kPa	348.50	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	3.21	kPa	350.90	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	4.16	kPa	356.10	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.33	kPa	310.70	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.25	kPa	305.70	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.21	kPa	303.70	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.17	kPa	300.70	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.17	kPa	300.50	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.12	kPa	295.10	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.10	kPa	292.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.08	kPa	288.80	Vapour pressures and enthalpies of vaporisation of alkyl formamides

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51271e+01
Coeff. B	-4.03766e+03
Coeff. C	-6.64310e+01
Temperature range (K), min.	338.52
Temperature range (K), max.	477.78

Sources

Vapour pressures and enthalpies of vaporisation of alkyl formamides:	https://www.doi.org/10.1016/j.fluid.2019.04.036
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and Correlation of Solubilities and Solution Thermodynamics for N,N-Diethylformamide + MCl (M = Na, K, Rb, and Cs) + Water Systems in the Temperature Range 288.15–338.15 K:	https://www.doi.org/10.1021/acs.jced.5b01043
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Solubility of 1,1-diamino-2,2-dinitroethylene in different pure solvents and binary mixtures (dimethyl sulfoxide p water) and (N,N-dimethylformamide p water) at different temperatures:	https://www.doi.org/10.1016/j.fluid.2017.12.035
Mackay Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C617845&Units=SI

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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume