

Formamide, N-butyl-

Other names:	Butylformamide Formamide, N-n-butyl- N-butyl-formamide N-butylformamide N-n-Butylformamide
Inchi:	InChI=1S/C5H11NO/c1-2-3-4-6-5-7/h5H,2-4H2,1H3,(H,6,7)
InchiKey:	QQGNLKJAIVSNCO-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CCCCNC=O
Mol. weight [g/mol]:	101.15
CAS:	871-71-6

Physical Properties

Property code	Value	Unit	Source
gf	-18.91	kJ/mol	Joback Method
hf	-178.64	kJ/mol	Joback Method
hfus	16.09	kJ/mol	Joback Method
hvap	39.88	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	0.532		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	1067.00		NIST Webbook
rinpol	1067.00		NIST Webbook
tb	412.63	K	Joback Method
tc	590.94	K	Joback Method
tf	240.77	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.95	J/molxK	590.94	Joback Method
cpg	224.45	J/molxK	561.22	Joback Method

cpg	216.62	J/mol×K	531.50	Joback Method
cpg	208.43	J/mol×K	501.78	Joback Method
cpg	199.89	J/mol×K	472.07	Joback Method
cpg	190.97	J/mol×K	442.35	Joback Method
cpg	181.67	J/mol×K	412.63	Joback Method
pvap	0.05	kPa	331.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.01	kPa	316.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.02	kPa	317.80	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.02	kPa	318.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.02	kPa	320.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.03	kPa	323.10	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.03	kPa	326.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.04	kPa	329.10	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.01	kPa	314.10	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.06	kPa	334.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides

pvap	0.08	kPa	337.10	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.09	kPa	340.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.12	kPa	343.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.14	kPa	346.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.17	kPa	349.10	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	0.21	kPa	352.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	9.12e-03	kPa	310.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	7.31e-03	kPa	307.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	5.60e-03	kPa	304.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	4.22e-03	kPa	301.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	3.49e-03	kPa	299.30	Vapour pressures and enthalpies of vaporisation of alkyl formamides
pvap	3.21e-03	kPa	298.20	Vapour pressures and enthalpies of vaporisation of alkyl formamides

pvap

2.93e-03

kPa

297.10

Vapour pressures and enthalpies of vaporisation of alkyl formamides

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vaporisation of alkyl formamides:	https://www.doi.org/10.1016/j.fluid.2019.04.036
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=C871716&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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