Acetamide, N,N-dibutyl-

Other names:	N,N-Dibutylacetamide
	N,N-di-n-Butylacetamide
Inchi:	InChI=1S/C10H21NO/c1-4-6-8-11(10(3)12)9-7-5-2/h4-9H2,1-3H3
InchiKey:	MEXKFCWMWJZDMF-UHFFFAOYSA-N
Formula:	C10H21NO
SMILES:	CCCCN(CCCC)C(C)=O
Mol. weight [g/mol]:	171.28
CAS:	1563-90-2

Physical Properties

Property code	Value	Unit	Source
gf	15.18	kJ/mol	Joback Method
hf	-294.78	kJ/mol	Joback Method
hfus	26.28	kJ/mol	Joback Method
hvap	46.64	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.435		Crippen Method
mcvol	163.310	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	1332.00		NIST Webbook
rinpol	1332.00		NIST Webbook
ripol	1808.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1813.00		NIST Webbook
ripol	1813.00		NIST Webbook
ripol	1805.00		NIST Webbook
ripol	1805.00		NIST Webbook
tb	494.51	K	Joback Method
tc	665.67	K	Joback Method
tf	284.86	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.88	J/mol×K	494.51	Joback Method
cpg	391.01	J/mol×K	523.04	Joback Method
cpg	405.50	J/mol×K	551.56	Joback Method
cpg	419.35	J/mol×K	580.09	Joback Method
cpg	432.59	J/mol×K	608.62	Joback Method
cpg	445.24	J/mol×K	637.14	Joback Method
cpg	457.30	J/mol×K	665.67	Joback Method
pvap	0.01	kPa	317.50	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	2.47e-03	kPa	298.80	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	2.92e-03	kPa	300.90	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	3.24e-03	kPa	301.80	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	4.02e-03	kPa	303.90	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	5.05e-03	kPa	306.60	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	5.14e-03	kPa	306.70	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	6.35e-03	kPa	308.80	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	8.44e-03	kPa	312.50	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides

pvap	0.01	kPa	315.70	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	1.30e-03	kPa	291.80	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.02	kPa	320.40	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.02	kPa	320.70	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.02	kPa	320.80	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.02	kPa	322.60	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.02	kPa	323.60	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.02	kPa	325.60	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.03	kPa	327.20	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.03	kPa	327.60	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.03	kPa	330.60	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.04	kPa	330.60	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides

pvap	0.04	kPa	333.30	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.05	kPa	334.80	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.05	kPa	335.70	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.06	kPa	337.50	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.07	kPa	340.70	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.09	kPa	343.60	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65907e+01
Coeff. B	-5.11457e+03
Coeff. C	-8.70030e+01
Temperature range (K), min.	400.72
Temperature range (K), max.	540.45

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1563902&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides:	https://www.doi.org/10.1016/j.fluid.2019.112241
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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