

Acetamide, N,N-diethyl-

Other names:	CH3CON(C2H5)2 N,N-Diethylacetamide N,N-diethylethanamide
Inchi:	InChI=1S/C6H13NO/c1-4-7(5-2)6(3)8/h4-5H2,1-3H3
InchiKey:	AJFDBNQDYLMJN-UHFFFAOYSA-N
Formula:	C6H13NO
SMILES:	CCN(CC)C(C)=O
Mol. weight [g/mol]:	115.17
CAS:	685-91-6

Physical Properties

Property code	Value	Unit	Source
affp	925.40	kJ/mol	NIST Webbook
basg	894.40	kJ/mol	NIST Webbook
chl	-3883.60 ± 3.20	kJ/mol	NIST Webbook
gf	-18.50	kJ/mol	Joback Method
hf	-287.20	kJ/mol	NIST Webbook
hfl	-335.40 ± 3.20	kJ/mol	NIST Webbook
hfus	53.70	kJ/mol	Enthalpies of vaporization of N,N-dialkyl monamides at 298.15K
hvap	48.20	kJ/mol	NIST Webbook
ie	8.60 ± 0.02	eV	NIST Webbook
log10ws	-0.68		Crippen Method
logp	0.875		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	966.00		NIST Webbook
rinpol	985.00		NIST Webbook
ripol	1595.00		NIST Webbook
tb	457.20	K	NIST Webbook
tc	578.97	K	Joback Method
tf	239.78	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.41	J/mol×K	402.99	Joback Method
cpg	216.70	J/mol×K	432.32	Joback Method
cpg	227.51	J/mol×K	461.65	Joback Method
cpg	237.84	J/mol×K	490.98	Joback Method
cpg	247.72	J/mol×K	520.31	Joback Method
cpg	257.15	J/mol×K	549.64	Joback Method
cpg	266.15	J/mol×K	578.97	Joback Method
pvap	0.10	kPa	300.70	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.06	kPa	295.70	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.08	kPa	298.10	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.05	kPa	293.20	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.11	kPa	303.30	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.16	kPa	308.20	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.18	kPa	310.60	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.22	kPa	313.20	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides

pvap	0.31	kPa	318.20	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.42	kPa	323.30	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.50	kPa	325.70	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.59	kPa	328.20	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.68	kPa	330.70	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides
pvap	0.81	kPa	333.10	Vapour pressures and enthalpies of vaporisation of N,N-di-alkylacetamides

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56855e+01
Coeff. B	-4.30011e+03
Coeff. C	-6.86550e+01
Temperature range (K), min.	347.92
Temperature range (K), max.	483.16

Sources

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>

Enthalpies of vaporization of
N,N-dialkyl monamides at 298.15K:
Joback Method:

<https://www.doi.org/10.1016/j.tca.2009.05.007>

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=C685916&Units=SI>

The Yaws Handbook of Vapor
Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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
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

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