

Acetamide, N-ethyl-

Other names:	Acetamidoethane Ethylacetamide N-Ethylacetamide N-Acetyethylamine Acetoethylamide N-Aethylacetamid
Inchi:	InChI=1S/C4H9NO/c1-3-5-4(2)6/h3H2,1-2H3,(H,5,6)
InchiKey:	PMDCZENCAXMSOU-UHFFFAOYSA-N
Formula:	C4H9NO
SMILES:	CCNC(C)=O
Mol. weight [g/mol]:	87.12
CAS:	625-50-3

Physical Properties

Property code	Value	Unit	Source
affp	898.00	kJ/mol	NIST Webbook
basg	867.00	kJ/mol	NIST Webbook
gf	-56.73	kJ/mol	Joback Method
hf	-185.00	kJ/mol	Joback Method
hfus	12.81	kJ/mol	Joback Method
hvap	64.90 ± 0.20	kJ/mol	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
log10ws	-0.46		Crippen Method
logp	0.142		Crippen Method
mcvol	78.770	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
rinpol	877.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	890.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1608.00		NIST Webbook
tb	478.20	K	NIST Webbook
tc	579.58	K	Joback Method
tf	237.43	K	Joback Method
vc	0.300	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.48	J/mol×K	394.96	Joback Method
cpg	151.71	J/mol×K	425.73	Joback Method
cpg	159.61	J/mol×K	456.50	Joback Method
cpg	167.19	J/mol×K	487.27	Joback Method
cpg	174.45	J/mol×K	518.04	Joback Method
cpg	181.39	J/mol×K	548.81	Joback Method
cpg	188.03	J/mol×K	579.58	Joback Method
cpl	180.28	J/mol×K	298.15	NIST Webbook
cpl	180.00	J/mol×K	298.15	NIST Webbook
hvapt	55.70	kJ/mol	392.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.20	K	1.00	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C625503&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

affp: Proton affinity

basg: Gas basicity

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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

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