N-Acetylethylenediamine

Other names:	Acetamide, N-(2-aminoethyl)-
	Acetamide, N-(2-aminoethyl-)
	N-Monoacetylethylenediamine
Inchi:	InChI=1S/C4H10N2O/c1-4(7)6-3-2-5/h2-3,5H2,1H3,(H,6,7)
InchiKey:	DAKZISABEDGGSV-UHFFFAOYSA-N
Formula:	C4H10N2O
SMILES:	CC(=O)NCCN
Mol. weight [g/mol]:	102.14
CAS:	1001-53-2

Physical Properties

Property code	Value	Unit	Source
hfus	18.01	kJ/mol	Joback Method
hvap	61.58	kJ/mol	Cheméo Relay (1.0)
ie	9.20	eV	Cheméo Relay (1.0)
logp	-0.919		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
tb	496.84	K	Cheméo Relay (1.0)
tf	320.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	401.20	K	0.40	NIST Webbook

Correlations

Information	Value
Property code	cpg

Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	1.18920e+01
Coeff. B	4.93920e-01
Coeff. C	-2.67100e-04
Coeff. D	4.88600e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1001532&Units=SI

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point

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