1,2-Ethanediamine, N-propyl-

Other names: Ethylenediamine, N-propyl-
N-Propylethylenediamine
N-n-Propylethylenediamine
Inchi: InChI=1S/C5H14N2/c1-2-4-7-5-3-6/h7H,2-6H2,1H3
InchiKey: CFNHVUGPXZUTRR-UHFFFAOYSA-N
Formula: C5H14N2
SMILES: CCCNCCN
Mol. weight [g/mol]: 102.18
CAS: 111-39-7

Physical Properties

Property code	Value	Unit	Source
gf	147.06	kJ/mol	Joback Method
hf	-59.27	kJ/mol	Joback Method
hfus	19.00	kJ/mol	Joback Method
hvap	43.80	kJ/mol	Joback Method
log10ws	-0.54		Crippen Method
logp	-0.055		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	421.70	K	NIST Webbook
tc	621.90	K	Joback Method
tf	282.03	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.90	J/mol×K	436.50	Joback Method
cpg	224.78	J/mol×K	467.40	Joback Method
cpg	235.20	J/mol×K	498.30	Joback Method
cpg	245.17	J/mol×K	529.20	Joback Method
cpg	254.70	J/mol×K	560.10	Joback Method
cpg	263.81	J/mol×K	591.00	Joback Method

cpg	272.50	J/mol×K	621.90	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56567e+01
Coeff. B	-4.01059e+03
Coeff. C	-5.83690e+01
Temperature range (K), min.	319.32
Temperature range (K), max.	446.04

Sources

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
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=C111397&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
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume