

2-Amino-2-ethyl-1,3-propanediol

Other names:	1,3-Propanediol, 2-amino-2-ethyl- 2-Amino-1,3-dihydroxy-2-ethylpropane 2-Ethyl-2-aminopropanediol 2-amino-2-ethylpropanediol AEPD AEPD-85 Aminoethyl propanediol
Inchi:	InChI=1S/C5H13NO2/c1-2-5(6,3-7)4-8/h7-8H,2-4,6H2,1H3
InchiKey:	IOAOAKDONABGPZ-UHFFFAOYSA-N
Formula:	C5H13NO2
SMILES:	CCC(N)(CO)CO
Mol. weight [g/mol]:	119.16
CAS:	115-70-8

Physical Properties

Property code	Value	Unit	Source
gf	-213.13	kJ/mol	Joback Method
hf	-425.95	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	69.43	kJ/mol	Joback Method
log10ws	0.01		Crippen Method
logp	-0.921		Crippen Method
mcvol	103.030	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
tb	567.46	K	Joback Method
tc	743.97	K	Joback Method
tf	309.00 ± 1.00	K	NIST Webbook
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.51	J/mol×K	567.46	Joback Method
cpg	274.68	J/mol×K	596.88	Joback Method

cpg	282.40	J/mol×K	626.30	Joback Method
cpg	289.71	J/mol×K	655.71	Joback Method
cpg	296.62	J/mol×K	685.13	Joback Method
cpg	303.16	J/mol×K	714.55	Joback Method
cpg	309.36	J/mol×K	743.97	Joback Method
cpl	374.10	J/mol×K	313.15	Molar heat capacities of aqueous 2-amino-2-ethyl-1,3-propanediol solutions and their ternary mixtures containing piperazine or lithium salts
cpl	370.50	J/mol×K	308.15	Molar heat capacities of aqueous 2-amino-2-ethyl-1,3-propanediol solutions and their ternary mixtures containing piperazine or lithium salts
cpl	367.50	J/mol×K	303.15	Molar heat capacities of aqueous 2-amino-2-ethyl-1,3-propanediol solutions and their ternary mixtures containing piperazine or lithium salts
cpl	378.00	J/mol×K	318.15	Molar heat capacities of aqueous 2-amino-2-ethyl-1,3-propanediol solutions and their ternary mixtures containing piperazine or lithium salts
cpl	381.50	J/mol×K	323.15	Molar heat capacities of aqueous 2-amino-2-ethyl-1,3-propanediol solutions and their ternary mixtures containing piperazine or lithium salts

cpl	385.80	J/mol×K	328.15	Molar heat capacities of aqueous 2-amino-2-ethyl-1,3-propanediol solutions and their ternary mixtures containing piperazine or lithium salts
cpl	389.90	J/mol×K	333.15	Molar heat capacities of aqueous 2-amino-2-ethyl-1,3-propanediol solutions and their ternary mixtures containing piperazine or lithium salts
cpl	393.90	J/mol×K	338.15	Molar heat capacities of aqueous 2-amino-2-ethyl-1,3-propanediol solutions and their ternary mixtures containing piperazine or lithium salts
cpl	398.60	J/mol×K	343.15	Molar heat capacities of aqueous 2-amino-2-ethyl-1,3-propanediol solutions and their ternary mixtures containing piperazine or lithium salts
cpl	403.10	J/mol×K	348.15	Molar heat capacities of aqueous 2-amino-2-ethyl-1,3-propanediol solutions and their ternary mixtures containing piperazine or lithium salts
cpl	408.20	J/mol×K	353.15	Molar heat capacities of aqueous 2-amino-2-ethyl-1,3-propanediol solutions and their ternary mixtures containing piperazine or lithium salts

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	425.00	K	1.30	NIST Webbook
tbrp	419.00	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47386e+01
Coeff. B	-4.24422e+03
Coeff. C	-6.62220e+01
Temperature range (K), min.	359.92
Temperature range (K), max.	516.44

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115708&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
Molar heat capacities of aqueous 2-amino-2-ethyl-1,3-propanediol Joback Method:	https://www.doi.org/10.1016/j.fluid.2013.12.017
Solutions and their ternary mixtures containing piperazine or lithium salts: 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
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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