2-Amino-2-methyl-1,3-propanediol

Other names:	1,1-Di(hydroxymethyl)ethylamine
	1,3-Dihydroxy-2-amino-2-methylpropane
	1,3-Dihydroxy-2-methyl-2-propylamine
	1,3-Propanediol, 2-amino-2-methyl-
	2-Amino-2-methylpropan-1,3-diol
	2-Amino-2-methylpropane-1,3-diol
	AMPD
	Aminoglycol
	Gentimon
	Isobutandiol-2-amine
	NSC 6364
Inchi:	InChI=1S/C4H11NO2/c1-4(5,2-6)3-7/h6-7H,2-3,5H2,1H3
InchiKey:	UXFQFBNBSPQBJW-UHFFFAOYSA-N
Formula:	C4H11NO2
SMILES:	CC(N)(CO)CO
Mol. weight [g/mol]:	105.14
CAS:	115-69-5

Physical Properties

Property code	Value	Unit	Source
gf	-221.55	kJ/mol	Joback Method
hf	-405.31	kJ/mol	Joback Method
hfus	23.55	kJ/mol	Heat capacity measurement of organic thermal energy storage materials
hvap	67.20	kJ/mol	Joback Method
log10ws	0.43		Crippen Method
logp	-1.312		Crippen Method
mcvol	88.940	ml/mol	McGowan Method
pc	5552.58	kPa	Joback Method
tb	544.58	K	Joback Method
tc	722.63	K	Joback Method
tf	384.00 ± 2.00	K	NIST Webbook
tt	384.08 ± 0.05	K	NIST Webbook
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.23	J/mol×K	544.58	Joback Method
cpg	237.32	J/mol×K	603.93	Joback Method
cpg	243.78	J/mol×K	633.61	Joback Method
cpg	249.88	J/mol×K	663.28	Joback Method
cpg	255.64	J/mol×K	692.96	Joback Method
cpg	261.08	J/mol×K	722.63	Joback Method
cpg	230.48	J/mol×K	574.26	Joback Method
cps	161.37	J/mol×K	301.40	NIST Webbook
hfust	5.00	kJ/mol	352.90	NIST Webbook
hfust	2.73	kJ/mol	383.60	NIST Webbook
hfust	2.78	kJ/mol	384.10	NIST Webbook
hfust	24.68	kJ/mol	351.30	NIST Webbook
hfust	2.99	kJ/mol	384.00	NIST Webbook
hfust	25.21	kJ/mol	352.00	NIST Webbook
hfust	2.78	kJ/mol	338.00	NIST Webbook
hfust	2.99	kJ/mol	384.00	NIST Webbook
hfust	18.46	kJ/mol	353.70	NIST Webbook
hfust	2.76	kJ/mol	384.10	NIST Webbook
sfust	7.24	J/mol×K	384.10	NIST Webbook
sfust	52.19	J/mol×K	353.70	NIST Webbook
sfust	14.17	J/mol×K	352.90	NIST Webbook
sfust	7.12	J/mol×K	383.60	NIST Webbook
sfust	7.79	J/mol×K	384.00	NIST Webbook
sfust	71.61	J/mol×K	352.00	NIST Webbook
sfust	70.26	J/mol×K	351.30	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	424.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	4.06801e+01
Coeff. B	-1.34550e+04
Coeff. C	-8.72100e+01
Temperature range (K), min.	420.32
Temperature range (K), max.	467.63

Sources

Heat capacity measurement of organic thermal energy storage materials:	https://www.doi.org/10.1016/j.jct.2006.02.005
Density and refractive index measurements of transition temperature mixture (deep eutectic analogues) based on potassium carbonate with dual hydrogen bond donors for CO2 capture:	https://www.doi.org/10.1016/j.jct.2017.11.008
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=C115695&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

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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