

2-Propanol, 1-(dimethylamino)-

Other names:	(+)-1-(dimethylamino)-2-propanol 1,1-(Dimethylamino)propanol-2 1,1-Dimethylaminopropan-2-ol 1-(Dimethylamino)-2-propanol 1-(Dimethylamino)propan-2-ol 2-(Dimethylamino)-1-methylethanol 2-Propanol, 1,1-(dimethylamino)- 3-Dimethylamino-2-propanol DL-1-(dimethylamino)-2-propanol Dimepranol Dimethyl(2-hydroxypropyl)amine Dimethylisopropanolamine INN N,N-(Dimethylamino)-2-propanol N,N-Dimethyl-2-hydroxypropylamine N,N-Dimethylisopropanolamine NSC 3163
Inchi:	InChI=1S/C5H13NO/c1-5(7)4-6(2)3/h5,7H,4H2,1-3H3
InchiKey:	NCXUNZWLEYGQAH-UHFFFAOYSA-N
Formula:	C5H13NO
SMILES:	CC(O)CN(C)C
Mol. weight [g/mol]:	103.16
CAS:	108-16-7

Physical Properties

Property code	Value	Unit	Source
gf	-37.26	kJ/mol	Joback Method
hf	-236.51	kJ/mol	Joback Method
hfus	12.29	kJ/mol	Joback Method
hvap	45.06	kJ/mol	Joback Method
log10ws	0.14		Crippen Method
logp	-0.071		Crippen Method
mcvol	97.160	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
tb	397.20	K	NIST Webbook
tc	581.92	K	Joback Method
tf	224.40	K	Joback Method

vc	0.346	m3/kmol	Joback Method
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.91	J/mol×K	417.98	Joback Method
cpg	234.40	J/mol×K	527.28	Joback Method
cpg	225.85	J/mol×K	499.95	Joback Method
cpg	216.93	J/mol×K	472.63	Joback Method
cpg	250.40	J/mol×K	581.92	Joback Method
cpg	207.62	J/mol×K	445.30	Joback Method
cpg	242.58	J/mol×K	554.60	Joback Method
rhoI	840.40	kg/m3	303.15	Density Measurements of Unloaded and CO2-Loaded 1-Dimethylamino-2-propanol at Temperatures (298.15 to 353.15) K
rhoI	835.60	kg/m3	308.15	Density Measurements of Unloaded and CO2-Loaded 1-Dimethylamino-2-propanol at Temperatures (298.15 to 353.15) K
rhoI	830.70	kg/m3	313.15	Density Measurements of Unloaded and CO2-Loaded 1-Dimethylamino-2-propanol at Temperatures (298.15 to 353.15) K
rhoI	825.90	kg/m3	318.15	Density Measurements of Unloaded and CO2-Loaded 1-Dimethylamino-2-propanol at Temperatures (298.15 to 353.15) K
rhoI	820.90	kg/m3	323.15	Density Measurements of Unloaded and CO2-Loaded 1-Dimethylamino-2-propanol at Temperatures (298.15 to 353.15) K

rhoI	845.20	kg/m3	298.15	Density Measurements of Unloaded and CO2-Loaded 1-Dimethylamino-2-propanol at Temperatures (298.15 to 353.15) K	
srf	0.02	N/m	323.20	Analysis of Surface Thermodynamics for Amino Acid Ionic Liquid-1-Dimethylamino-2-propanol Aqueous Blends	
srf	0.02	N/m	318.20	Analysis of Surface Thermodynamics for Amino Acid Ionic Liquid-1-Dimethylamino-2-propanol Aqueous Blends	
srf	0.02	N/m	313.20	Analysis of Surface Thermodynamics for Amino Acid Ionic Liquid-1-Dimethylamino-2-propanol Aqueous Blends	
srf	0.02	N/m	303.20	Analysis of Surface Thermodynamics for Amino Acid Ionic Liquid-1-Dimethylamino-2-propanol Aqueous Blends	
srf	0.02	N/m	323.20	Surface thermodynamics of DMA2P, DMA2P-MEA and DMA2P-PZ aqueous solutions	
srf	0.02	N/m	313.20	Surface thermodynamics of DMA2P, DMA2P-MEA and DMA2P-PZ aqueous solutions	
srf	0.02	N/m	303.20	Surface thermodynamics of DMA2P, DMA2P-MEA and DMA2P-PZ aqueous solutions	

srf	0.02	N/m	308.20	Analysis of Surface Thermodynamics for Amino Acid Ionic Liquid-1-Dimethylamino-2-propanol Aqueous Blends
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61920e+01
Coeff. B	-3.99873e+03
Coeff. C	-5.16970e+01
Temperature range (K), min.	302.99
Temperature range (K), max.	419.21

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Density Measurements of Unloaded and CO2-Loaded N-Dimethylamino-2-propanol at Temperatures (298.15 to 353.15) K: Surface thermodynamics of DMA2P, DMA2P-MEA and DMA2P-PZ aqueous solutions	https://www.doi.org/10.1021/je501126j
NIST-Webbook	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108167&Units=SI
Crippen Method:	https://www.doi.org/10.1016/j.jct.2016.12.022
Analysis of Surface Thermodynamics for Amino Acid Ionic Liquid-1-Dimethylamino-2-propanol Aqueous Blends:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.doi.org/10.1021/acs.jced.9b00511
Crippen Method:	http://link.springer.com/article/10.1007/BF02311772
	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rho:	Liquid Density
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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