1-Propanol, 3-(diethylamino)-

Other names:	3-(Diethylamino)-1-propanol
	3-(Diethylamino)propanol
	3-(Diethylamino)propyl alcohol
	3-diethylamino-1-propanol
	3-diethylaminopropan-1-ol
	Diethylpropanolamine
	N,N-Diethyl-3-hydroxypropylamine
	«gamma»-Diaethylaminopropanol
	Â«gammaÂ»-Diaethylaminopropanol
Inchi:	InChI=1S/C7H17NO/c1-3-8(4-2)6-5-7-9/h9H,3-7H2,1-2H3
InchiKey:	WKCYFSZDBICRKL-UHFFFAOYSA-N
Formula:	C7H17NO
SMILES:	CCN(CC)CCCO
Mol. weight [g/mol]:	131.22
CAS:	622-93-5

Physical Properties

Property code	Value	Unit	Source
gf	-17.98	kJ/mol	Joback Method
hf	-272.51	kJ/mol	Joback Method
hfus	21.00	kJ/mol	Joback Method
hvap	49.90	kJ/mol	Joback Method
ie	8.56 ± 0.05	eV	NIST Webbook
log10ws	-0.59		Crippen Method
logp	0.711		Crippen Method
mcvol	125.340	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	462.60	K	NIST Webbook
tb	462.70	K	NIST Webbook
tc	623.43	K	Joback Method
tf	261.94	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.08	J/mol×K	464.18	Joback Method
cpg	290.52	J/mol×K	490.72	Joback Method
cpg	301.50	J/mol×K	517.26	Joback Method
cpg	312.03	J/mol×K	543.81	Joback Method
cpg	322.14	J/mol×K	570.35	Joback Method
cpg	331.83	J/mol×K	596.89	Joback Method
cpg	341.12	J/mol×K	623.43	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	353.90	K	1.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	360.20	K	2.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	405.30	K	19.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture

tbp	409.20	K	22.30	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	412.10	K	24.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	420.20	K	34.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	427.30	K	44.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	433.40	K	54.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	440.10	K	64.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture
tbp	442.20	K	69.80	Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture

tbrp	355.20	K	2.00	NIST Webbook
tbrp	357.00	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61055e+01
Coeff. B	-4.51369e+03
Coeff. C	-6.97670e+01
Temperature range (K), min.	355.12
Temperature range (K), max.	487.93

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour-liquid equilibrium study of tertiary amines, single and in blend with 3-(methylamino)propylamine, for post-combustion CO2 capture:	https://www.doi.org/10.1016/j.jct.2019.06.017
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=C622935&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

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
ie:	Ionization energy
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
tbp:	Boiling point at given pressure
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume