Triethylenediamine

Other names:	1,4 Diazabicyclo (2,2,2)octane
	1,4-Diaza[2.2.2]bicyclooctane
	1,4-Diazabicyclo[2.2.2]octane
	1,4-Ethylenepiperazine
	1,4-diazabicyclooctane
	BICYCLO[2.2.2]-1,4-DIAZAOCTANE
	Bicyclo[2.2.2]octane, 1,4-diaza-
	D 33LV
	DABCO
	Dabco 33LV
	Dabco Crystal
	Dabco R-8020
	Dabco S-25
	Dabco crystalline
	N,N'-ENDO-ETHYLENEPIPERAZINE
	NSC 56362
	TED
	TEDA
	TEDA-L33
	Tegoamin 33
	Texacat TD 100
	Texacat TD-33
Inchi:	InChI=1S/C6H12N2/c1-2-8-5-3-7(1)4-6-8/h1-6H2
InchiKey:	IMNIMPAHZVJRPE-UHFFFAOYSA-N
Formula:	C6H12N2
SMILES:	C1CN2CCN1CC2
Mol. weight [g/mol]:	112.17
CAS:	280-57-9

Physical Properties

Property code	Value	Unit	Source
log10ws	0.74		Crippen Method
logp	-0.382		Crippen Method
mcvol	93.640	ml/mol	McGowan Method
rinpol	1018.00		NIST Webbook
ripol	1520.00		NIST Webbook

tf	434.25	K	KDB
tf	432.45	K	Solubility of Triethylenediamine in Methanol, Ethanol, Isopropanol, I-Butanol, and Ethyl Acetate between 276.15 K and 363.15 K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44470e+01
Coeff. B	-3.45373e+03
Coeff. C	-9.57570e+01
Temperature range (K), min.	339.67
Temperature range (K), max.	473.81

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.48808e+02
Coeff. B	-1.23733e+04
Coeff. C	-1.94220e+01
Coeff. D	1.00224e-05
Temperature range (K), min.	323.15
Temperature range (K), max.	655.00

Sources

Solubility of Triethylenediamine in Methanol, Ethanol, Isopropanol, I-Butanol, and Ethyl Acetate between 276.15 K and 363.15 K:	https://www.doi.org/10.1021/je700186v
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1324
Vapor Liquid Equilibrium for Binary Mixtures of 1,4-Diazabicyclo[2.2.2]octane with Ethylenediamine, Ethanolamine, and Ethylene Glycol:	https://www.doi.org/10.1007/s10765-009-0570-x
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C280579&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1324.mol

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point