1-Propanamine, N,N-diethyl-

Other names:	(C2H5)2(n-C3H7)N
	Diethyl-n-propylamine
	Diethylpropylamine
	Ethanamine, N-ethyl-N-propyl-
	N,N-Diethyl-n-propylamine
	N-(n-Propyl)diethylamine
	Propylamine, N,N-diethyl-
	n-Propanamine, N,N-diethyl-
Inchi:	InChI=1S/C7H17N/c1-4-7-8(5-2)6-3/h4-7H2,1-3H3
InchiKey:	PQZTVWVYCLIIJY-UHFFFAOYSA-N
Formula:	C7H17N
SMILES:	CCCN(CC)CC
Mol. weight [g/mol]:	115.22
CAS:	4458-31-5

Physical Properties

Property code	Value	Unit	Source
affp	978.80	kJ/mol	NIST Webbook
basg	947.90	kJ/mol	NIST Webbook
gf	118.84	kJ/mol	Joback Method
hf	-120.28	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	33.22	kJ/mol	Joback Method
ie	7.70	eV	NIST Webbook
log10ws	-1.32		Crippen Method
logp	1.738		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	750.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	750.00		NIST Webbook
tb	404.15 ± 2.00	K	NIST Webbook
tb	385.20 ± 1.00	K	NIST Webbook
tc	534.55	K	Joback Method

tf	201.12	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.39	J/mol×K	372.00	Joback Method
cpg	234.38	J/mol×K	399.09	Joback Method
cpg	246.88	J/mol×K	426.18	Joback Method
cpg	258.89	J/mol×K	453.28	Joback Method
cpg	270.43	J/mol×K	480.37	Joback Method
cpg	281.51	J/mol×K	507.46	Joback Method
cpg	292.14	J/mol×K	534.55	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56364e+01
Coeff. B	-3.71285e+03
Coeff. C	-4.82220e+01
Temperature range (K), min.	290.12
Temperature range (K), max.	407.82

Sources

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=C4458315&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

affp:	Proton affinity
basg:	Gas basicity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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