Benzenamine, N-propyl-

Other names:	Aniline, N-n-propyl-
	Aniline, N-propyl-
	N-(n-Propyl)aniline
	N-Propylaniline
	Propylaniline
Inchi:	InChI=1S/C9H13N/c1-2-8-10-9-6-4-3-5-7-9/h3-7,10H,2,8H2,1H3
InchiKey:	CDZOGLJOFWFVOZ-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CCCNc1ccccc1
Mol. weight [g/mol]:	135.21
CAS:	622-80-0

Physical Properties

Property code	Value	Unit	Source
gf	226.70	kJ/mol	Joback Method
hf	60.91	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	44.34	kJ/mol	Joback Method
ie	7.54	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
log10ws	-2.32		Crippen Method
logp	2.508		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	495.20	K	NIST Webbook
tc	691.55	K	Joback Method
tf	270.27	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.33	J/mol×K	482.17	Joback Method
cpg	274.63	J/mol×K	517.07	Joback Method

cpg	288.10	J/mol×K	551.96	Joback Method
cpg	300.77	J/mol×K	586.86	Joback Method
cpg	312.68	J/mol×K	621.76	Joback Method
cpg	323.85	J/mol×K	656.66	Joback Method
cpg	334.34	J/mol×K	691.55	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.20	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48211e+01
Coeff. B	-4.24839e+03
Coeff. C	-7.88020e+01
Temperature range (K), min.	371.12
Temperature range (K), max.	525.55

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C622800&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume