

Benzenamine, 4-propyl-

Other names:	(p-Propylphenyl)amine 1-Amino-4-propylbenzene 4-Propylaniline 4-Propylbenzenamine 4-n-Propylaniline Aniline, 4-propyl- Aniline, p-propyl- NSC 13208 p-Aminopropylbenzene p-Propylaniline p-n-Propylaniline
Inchi:	InChI=1S/C9H13N/c1-2-3-8-4-6-9(10)7-5-8/h4-7H,2-3,10H2,1H3
InchiKey:	OAPDPORYXWQVJE-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CCCC1CCC(N)CC1
Mol. weight [g/mol]:	135.21
CAS:	2696-84-6

Physical Properties

Property code	Value	Unit	Source
gf	194.13	kJ/mol	Joback Method
hf	29.76	kJ/mol	Joback Method
hfus	17.92	kJ/mol	Joback Method
hvap	49.21	kJ/mol	Joback Method
ie	7.42	eV	NIST Webbook
ie	7.41	eV	NIST Webbook
log10ws	-2.33		Crippen Method
logp	2.221		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
ripol	1231.10		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2050.00		NIST Webbook
tb	498.20	K	NIST Webbook
tc	730.11	K	Joback Method
tf	313.39	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.53	J/mol×K	509.51	Joback Method
cpg	285.22	J/mol×K	546.28	Joback Method
cpg	298.11	J/mol×K	583.04	Joback Method
cpg	310.23	J/mol×K	619.81	Joback Method
cpg	321.61	J/mol×K	656.58	Joback Method
cpg	332.28	J/mol×K	693.35	Joback Method
cpg	342.28	J/mol×K	730.11	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	334.00 ± 1.00	K	0.07	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47433e+01
Coeff. B	-4.24074e+03
Coeff. C	-7.93580e+01
Temperature range (K), min.	372.72
Temperature range (K), max.	528.98

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=C2696846&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.cheméo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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