p-Pentylaniline

Other names:	4-Pentylaniline
	Benzenamine, 4-pentyl-
	p-n-Amylaniline
	p-n-Pentylaniline
Inchi:	InChI=1S/C11H17N/c1-2-3-4-5-10-6-8-11(12)9-7-10/h6-9H,2-5,12H2,1H3
InchiKey:	DGFTWBUZRHAHTH-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	CCCCCc1ccc(N)cc1
Mol. weight [g/mol]:	163.26
CAS:	33228-44-3

Physical Properties

Property code	Value	Unit	Source
gf	210.97	kJ/mol	Joback Method
hf	-11.52	kJ/mol	Joback Method
hfus	23.09	kJ/mol	Joback Method
hvap	53.66	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	3.002		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
tb	555.27	K	Joback Method
tc	768.54	K	Joback Method
tf	335.93	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.66	J/mol×K	555.27	Joback Method
cpg	378.10	J/mol×K	590.82	Joback Method
cpg	392.67	J/mol×K	626.36	Joback Method
cpg	406.38	J/mol×K	661.91	Joback Method
cpg	419.28	J/mol×K	697.45	Joback Method

cpg	431.41	J/mol×K	733.00	Joback Method
cpg	442.79	J/mol×K	768.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.50 ± 0.50	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51922e+01
Coeff. B	-4.62802e+03
Coeff. C	-8.84900e+01
Temperature range (K), min.	399.00
Temperature range (K), max.	556.88

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33228443&Units=SI

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
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