4-sec-Butylaniline

Other names:	4-Amino-sec-butylbenzene Aniline, p-sec-butyl- Benzenamine, 4-(1-methylpropyl)- p-sec-Butylaniline
Inchi:	InChI=1S/C10H15N/c1-3-8(2)9-4-6-10(11)7-5-9/h4-8H,3,11H2,1-2H3
InchiKey:	NVVVQTNTLIAISI-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CCC(C)c1ccc(N)cc1
Mol. weight [g/mol]:	149.23
CAS:	30273-11-1

Physical Properties

Property code	Value	Unit	Source
gf	200.11	kJ/mol	Joback Method
hf	3.84	kJ/mol	Joback Method
hfus	16.98	kJ/mol	Joback Method
hvap	51.05	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.782		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
tb	531.95	K	Joback Method
tc	753.77	K	Joback Method
tf	309.66	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.49	J/mol×K	531.95	Joback Method
cpg	331.53	J/mol×K	568.92	Joback Method
cpg	345.68	J/mol×K	605.89	Joback Method
cpg	358.96	J/mol×K	642.86	Joback Method
cpg	371.42	J/mol×K	679.83	Joback Method

cpg	383.09	J/mol×K	716.80	Joback Method
cpg	394.01	J/mol×K	753.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	517.70	K	96.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42580e+01
Coeff. B	-4.20048e+03
Coeff. C	-8.32500e+01
Temperature range (K), min.	383.92
Temperature range (K), max.	552.76

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=C30273111&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

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