

Benzenamine, 2-(1,1-dimethylethyl)-

Other names:	2-tert-Butylaniline Aniline, 2-tert-butyl-
Inchi:	InChI=1S/C10H15N/c1-10(2,3)8-6-4-5-7-9(8)11/h4-7H,11H2,1-3H3
InchiKey:	AEIOZWYBDBVCGW-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CC(C)(C)c1ccccc1N
Mol. weight [g/mol]:	149.23
CAS:	6310-21-0

Physical Properties

Property code	Value	Unit	Source
gf	205.39	kJ/mol	Joback Method
hf	0.37	kJ/mol	Joback Method
hfus	13.09	kJ/mol	Joback Method
hvap	62.70 ± 0.40	kJ/mol	NIST Webbook
log10ws	-2.42		Crippen Method
logp	2.566		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
tb	507.20	K	NIST Webbook
tc	760.46	K	Joback Method
tf	327.08	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.50	J/molxK	529.16	Joback Method
cpg	335.25	J/molxK	567.71	Joback Method
cpg	349.89	J/molxK	606.26	Joback Method
cpg	363.48	J/molxK	644.81	Joback Method
cpg	376.10	J/molxK	683.36	Joback Method
cpg	387.79	J/molxK	721.91	Joback Method
cpg	398.65	J/molxK	760.46	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	396.70	K	2.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48419e+01
Coeff. B	-4.34566e+03
Coeff. C	-8.21380e+01
Temperature range (K), min.	380.72
Temperature range (K), max.	538.11

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6310210&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/ci9903071
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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