Benzenemethanamine, N-(1,1-dimethylethyl)-

Other names:	N-Benzyl-tert-butylamine
	N-t-Butylbenzylamine
	N-tert-Butylbenzylamine
	tert-Butylbenzylamine
Inchi:	InChI=1S/C11H17N/c1-11(2,3)12-9-10-7-5-4-6-8-10/h4-8,12H,9H2,1-3H3
InchiKey:	DLSOILHAKCBARI-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	CC(C)(C)NCc1ccccc1
Mol. weight [g/mol]:	163.26
CAS:	3378-72-1

Physical Properties

Property code	Value	Unit	Source
gf	246.38	kJ/mol	Joback Method
hf	10.88	kJ/mol	Joback Method
hfus	15.97	kJ/mol	Joback Method
hvap	47.50	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.575		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
tb	524.70	K	Joback Method
tc	741.06	K	Joback Method
tf	295.23	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.65	J/mol×K	524.70	Joback Method
cpg	370.82	J/mol×K	560.76	Joback Method
cpg	386.85	J/mol×K	596.82	Joback Method
cpg	401.78	J/mol×K	632.88	Joback Method
cpg	415.69	J/mol×K	668.94	Joback Method

cpg	428.64	J/mol×K	705.00	Joback Method
cpg	440.70	J/mol×K	741.06	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.20	K	0.70	NIST Webbook
tbrp	374.00 ± 1.00	K	2.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40687e+01
Coeff. B	-4.15058e+03
Coeff. C	-8.43200e+01
Temperature range (K), min.	385.50
Temperature range (K), max.	558.28

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=C3378721&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

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