N-Butylbenzylamine

Other names:	Benzenemethanamine, N-butyl-
	Benzylamine, N-butyl-
	Benzylbutylamine
	Butylbenzylamine
	N-(n-Butyl)benzylamine
	N-Benzyl-N-butylamine
	N-Benzylbutylamine
	NSC 15681
	NSC 32386
Inchi:	InChI=1S/C11H17N/c1-2-3-9-12-10-11-7-5-4-6-8-11/h4-8,12H,2-3,9-10H2,1H3
InchiKey:	HIPXPABRMMYVQD-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	CCCCNCc1ccccc1
Mol. weight [g/mol]:	163.26
CAS:	2403-22-7

Physical Properties

Property code	Value	Unit	Source
gf	243.54	kJ/mol	Joback Method
hf	19.63	kJ/mol	Joback Method
hfus	23.39	kJ/mol	Joback Method
hvap	48.79	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.576		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1302.50		NIST Webbook
rinpol	1302.50		NIST Webbook
ripol	1726.00		NIST Webbook
tb	527.93	K	Joback Method
tc	731.26	K	Joback Method
tf	292.81	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.57	J/mol×K	527.93	Joback Method
cpg	366.56	J/mol×K	561.82	Joback Method
cpg	381.64	J/mol×K	595.71	Joback Method
cpg	395.87	J/mol×K	629.60	Joback Method
cpg	409.26	J/mol×K	663.49	Joback Method
cpg	421.86	J/mol×K	697.37	Joback Method
cpg	433.71	J/mol×K	731.26	Joback Method

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

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=C2403227&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume