

Benzenamine, N,N-dibutyl-

Other names:	Aniline, N,N-dibutyl- Dibutylamine, N-phenyl- Dibutylaniline N,N-Dibutylaniline N,N-Dibutylbenzenamine N,N-di-n-Butylaniline N-Phenyldibutylamine
Inchi:	InChI=1S/C14H23N/c1-3-5-12-15(13-6-4-2)14-10-8-7-9-11-14/h7-11H,3-6,12-13H2,1-2H
InchiKey:	FZPXKEPZZOEPGX-UHFFFAOYSA-N
Formula:	C14H23N
SMILES:	CCCCN(CCCC)c1ccccc1
Mol. weight [g/mol]:	205.34
CAS:	613-29-6

Physical Properties

Property code	Value	Unit	Source
gf	290.19	kJ/mol	Joback Method
hf	-28.23	kJ/mol	Joback Method
hfus	29.08	kJ/mol	Joback Method
hvap	51.08	kJ/mol	Joback Method
ie	6.95	eV	NIST Webbook
ie	7.15	eV	NIST Webbook
log10ws	-3.89		Crippen Method
logp	4.093		Crippen Method
mcvol	194.340	ml/mol	McGowan Method
pc	2005.50	kPa	Joback Method
tb	542.65 ± 2.00	K	NIST Webbook
tb	542.70	K	NIST Webbook
tc	750.52	K	Joback Method
tf	241.00 ± 0.02	K	NIST Webbook
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.89	J/mol×K	558.84	Joback Method
cpg	497.48	J/mol×K	590.79	Joback Method
cpg	515.05	J/mol×K	622.73	Joback Method
cpg	531.66	J/mol×K	654.68	Joback Method
cpg	547.34	J/mol×K	686.62	Joback Method
cpg	562.15	J/mol×K	718.57	Joback Method
cpg	576.11	J/mol×K	750.52	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53290e+01
Coeff. B	-4.81143e+03
Coeff. C	-9.34800e+01
Temperature range (K), min.	413.36
Temperature range (K), max.	573.78

Sources

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=C613296&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

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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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