

Dibenzylamine

Other names:	(N-Benzylaminomethyl)benzene Accelerator DBA BENZENEMETHANAMINE Benzenemethanamine, N-(phenylmethyl)- Bibenzylamine DBA N,N-Dibenzylamine N-(Phenylmethyl)benzenemethanamine N-BENZYLBENZYLAMINE NSC 4811 Vulcaid 28 bis(phenylmethyl)amine
Inchi:	InChI=1S/C14H15N/c1-3-7-13(8-4-1)11-15-12-14-9-5-2-6-10-14/h1-10,15H,11-12H2
InchiKey:	BWLUMTFWVZZZND-UHFFFAOYSA-N
Formula:	C14H15N
SMILES:	c1ccc(CNCc2ccccc2)cc1
Mol. weight [g/mol]:	197.28
CAS:	103-49-1

Physical Properties

Property code	Value	Unit	Source
chl	-7786.00	kJ/mol	NIST Webbook
gf	381.21	kJ/mol	Joback Method
hf	194.24	kJ/mol	Joback Method
hfl	97.10	kJ/mol	NIST Webbook
hfus	25.20	kJ/mol	Joback Method
hvap	57.75	kJ/mol	Joback Method
ie	8.22	eV	NIST Webbook
log10ws	-4.07		Crippen Method
logp	2.976		Crippen Method
mcvol	170.580	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1688.90		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1688.90		NIST Webbook
ripol	2473.00		NIST Webbook
ripol	2473.00		NIST Webbook

ripol	2427.00		NIST Webbook
tb	573.20	K	NIST Webbook
tb	542.15 ± 1.00	K	NIST Webbook
tc	860.81	K	Joback Method
tf	247.55 ± 0.40	K	NIST Webbook
tf	246.55 ± 0.40	K	NIST Webbook
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.39	J/mol×K	662.84	Joback Method
cpg	508.44	J/mol×K	860.81	Joback Method
cpg	497.17	J/mol×K	821.22	Joback Method
cpg	484.90	J/mol×K	781.63	Joback Method
cpg	471.57	J/mol×K	742.03	Joback Method
cpg	457.10	J/mol×K	702.44	Joback Method
cpg	424.38	J/mol×K	623.25	Joback Method
hvapt	70.50	kJ/mol	482.00	NIST Webbook
rho1	933.60	kg/m3	413.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rho1	998.50	kg/m3	328.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rho1	994.60	kg/m3	333.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines

rhoI	990.80	kg/m3	338.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	986.90	kg/m3	343.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	983.10	kg/m3	348.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	979.30	kg/m3	353.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	975.40	kg/m3	358.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	971.60	kg/m3	363.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	967.80	kg/m3	368.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines

rhoI	964.00	kg/m3	373.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	960.20	kg/m3	378.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	956.40	kg/m3	383.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	952.60	kg/m3	388.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	948.80	kg/m3	393.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	945.00	kg/m3	398.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	941.20	kg/m3	403.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines

rhoI	937.40	kg/m3	408.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1002.40	kg/m3	323.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	929.80	kg/m3	418.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	926.00	kg/m3	423.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	922.20	kg/m3	428.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	918.50	kg/m3	433.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	914.60	kg/m3	438.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines

rhoI	910.80	kg/m3	443.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	907.00	kg/m3	448.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1026.48	kg/m3	293.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1022.59	kg/m3	298.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1018.70	kg/m3	303.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1014.82	kg/m3	308.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1010.94	kg/m3	313.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines

rhoI	1007.07	kg/m3	318.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1003.20	kg/m3	323.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	999.34	kg/m3	328.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	995.48	kg/m3	333.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	991.63	kg/m3	338.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	987.79	kg/m3	343.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1006.30	kg/m3	318.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines

rhoI	1010.20	kg/m3	313.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1014.20	kg/m3	308.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1018.10	kg/m3	303.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1022.20	kg/m3	298.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1026.20	kg/m3	293.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1030.30	kg/m3	288.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines
rhoI	1034.30	kg/m3	283.15	Measurement and Correlation for Acoustic, Transport, Refractive, and High-Temperature Volumetric Data of Substituted Benzylamines

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54236e+01
Coeff. B	-6.00192e+03
Coeff. C	-4.20810e+01
Temperature range (K), min.	438.61
Temperature range (K), max.	635.62

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.18547e+01
Coeff. B	-1.11806e+04
Coeff. C	-7.67012e+00
Coeff. D	3.00549e-06
Temperature range (K), min.	391.15
Temperature range (K), max.	573.15

Sources

KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1316
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103491&Units=SI
KDB:	https://www.thermo.com/files/research/kdb/mol/mol1316.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Measurement and Correlation for Acoustic, Transport, Refractive, and Dielectric Properties	https://www.doi.org/10.1021/acs.jced.6b00667
High Pressure Volumetric Data of Organic Compounds	https://www.chemed.com/doc/models/crippen_log10ws
Substituted Benzylamines:	http://link.springer.com/article/10.1007/BF02311772
McGowan Method:	

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
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

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