Benzyl nitrile

Other names:	(Cyanomethyl)benzene
	.alpha.-cyanotoluene
	.alpha.-phenylacetonitrile
	.alpha.-tolunitrile
	.omega.-cyanotoluene
	2-Phenylacetonitrile
	2-Phenylethanenitrile
	Acetonitrile, phenyl-
	Benzeneacetonitrile
	Benzyl cyanide
	NSC 118418
	Phenacetonitrile
	Phenyl acetonitrile
	Phenyl acetyl nitrile
	Phenylacetonitrile
	Toluene, «alpha»-cyano-
	Toluene, Â«alphaÂ»-cyano-
	UN 2470
	USAF KF-21
	benzylnitrile
	phenylethanenitrile
	«alpha»-Cyanotoluene
	«alpha»-Tolunitrile
	«omega»-Cyanotoluene
	Â«alphaÂ»-Cyanotoluene
	Â«alphaÂ»-Tolunitrile
	Â«omegaÂ»-Cyanotoluene
Inchi:	InChI=1S/C8H7N/c9-7-6-8-4-2-1-3-5-8/h1-5H,6H2
InchiKey:	SUSQOBVLVYHIEX-UHFFFAOYSA-N
Formula:	C8H7N
SMILES:	N#CCc1ccccc1
Mol. weight [g/mol]:	117.15
CAS:	140-29-4

Physical Properties

Property code	Value	Unit	Source

affp	805.50	kJ/mol	NIST Webbook
basg	774.80	kJ/mol	NIST Webbook
gf	262.07	kJ/mol	Joback Method
hf	192.96	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	60.50 ± 0.70	kJ/mol	NIST Webbook
ie	9.34	eV	NIST Webbook
ie	9.40 ± 0.05	eV	NIST Webbook
ie	9.50 ± 0.04	eV	NIST Webbook
ie	9.39 ± 0.07	eV	NIST Webbook
ie	9.32 ± 0.05	eV	NIST Webbook
log10ws	-2.14		Crippen Method
logp	1.753		Crippen Method
mcvol	101.200	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	1098.00		NIST Webbook
rinpol	1108.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1138.10		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1097.50		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1160.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1140.00		NIST Webbook

rinpol	1161.00	NIST Webbook
rinpol	1137.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1148.00	NIST Webbook
rinpol	1135.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1122.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1154.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1112.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1144.00	NIST Webbook
rinpol	1162.00	NIST Webbook
rinpol	1149.00	NIST Webbook
rinpol	1150.00	NIST Webbook
rinpol	1141.30	NIST Webbook
ripol	1941.00	NIST Webbook
ripol	1957.00	NIST Webbook
ripol	1947.00	NIST Webbook
ripol	1957.00	NIST Webbook
ripol	1893.00	NIST Webbook
ripol	1907.00	NIST Webbook
ripol	1920.00	NIST Webbook
ripol	1871.00	NIST Webbook
ripol	1871.00	NIST Webbook
ripol	1871.00	NIST Webbook
ripol	1910.00	NIST Webbook
ripol	1950.00	NIST Webbook
ripol	1946.00	NIST Webbook
ripol	1896.00	NIST Webbook
ripol	1947.00	NIST Webbook
ripol	1931.00	NIST Webbook
ripol	1901.00	NIST Webbook
ripol	1877.00	NIST Webbook
ripol	1927.00	NIST Webbook
ripol	1893.00	NIST Webbook
ripol	1902.00	NIST Webbook
ripol	1893.00	NIST Webbook
ripol	1890.00	NIST Webbook
ripol	1938.00	NIST Webbook

ripol	1907.00		NIST Webbook
ripol	1919.00		NIST Webbook
tb	506.70	K	NIST Webbook
tb	505.60 ± 0.60	K	NIST Webbook
tb	506.00 ± 0.50	K	NIST Webbook
tb	506.67 ± 0.30	K	NIST Webbook
tb	506.65 ± 0.50	K	NIST Webbook
tb	506.65 ± 1.00	K	NIST Webbook
tb	501.20 ± 3.00	K	NIST Webbook
tc	742.87	K	Joback Method
tf	250.71 ± 0.30	K	NIST Webbook
tf	251.15 ± 0.20	K	NIST Webbook
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.73	J/mol×K	511.20	Joback Method
cpg	212.16	J/mol×K	549.81	Joback Method
cpg	254.23	J/mol×K	742.87	Joback Method
cpg	247.04	J/mol×K	704.26	Joback Method
cpg	239.28	J/mol×K	665.65	Joback Method
cpg	230.90	J/mol×K	627.04	Joback Method
cpg	221.87	J/mol×K	588.42	Joback Method
dvisc	0.0016021	Pa×s	308.15	Volumetric and Transport Properties of Binary Liquid Mixtures of Phenylacetonitrile with Aliphatic Esters at Temperatures of (303.15 to 313.15) K
dvisc	0.0014893	Pa×s	313.15	Volumetric and Transport Properties of Binary Liquid Mixtures of Phenylacetonitrile with Aliphatic Esters at Temperatures of (303.15 to 313.15) K

dvisc	0.0017613	Pa×s	303.15	Volumetric and Transport Properties of Binary Liquid Mixtures of Phenylacetonitrile with Aliphatic Esters at Temperatures of (303.15 to 313.15) K
hvapt	54.80	kJ/mol	420.00	NIST Webbook
hvapt	60.10 ± 0.70	kJ/mol	305.50	NIST Webbook
rhol	1004.10	kg/m3	308.15	Excess Molar Volumes and Sound Speed in (Phenylacetonitrile + 1,2-Dichloroethane), (Phenylacetonitrile + 1,1,2-Trichloroethane), (Phenylacetonitrile + 1,1,2,2-Tetrachloroethane), (Phenylacetonitrile + Trichloroethene), and (Phenylacetonitrile + Tetrachloroethene) at Temperatures of (303.15, 308.15, and 313.15) K
rhol	1008.80	kg/m3	303.15	Excess Molar Volumes and Sound Speed in (Phenylacetonitrile + 1,2-Dichloroethane), (Phenylacetonitrile + 1,1,2-Trichloroethane), (Phenylacetonitrile + 1,1,2,2-Tetrachloroethane), (Phenylacetonitrile + Trichloroethene), and (Phenylacetonitrile + Tetrachloroethene) at Temperatures of (303.15, 308.15, and 313.15) K

rhol	1008.83	kg/m3	303.15	Excess Molar Volumes and Sound Speed in (Phenylacetonitrile + 1,2-Dichloroethane), (Phenylacetonitrile + 1,1,2-Trichloroethane), (Phenylacetonitrile + 1,1,2,2-Tetrachloroethane), (Phenylacetonitrile + Trichloroethene), and (Phenylacetonitrile + Tetrachloroethene) at Temperatures of (303.15, 308.15, and 313.15) K
rhol	999.50	kg/m3	313.15	Excess Molar Volumes and Sound Speed in (Phenylacetonitrile + 1,2-Dichloroethane), (Phenylacetonitrile + 1,1,2-Trichloroethane), (Phenylacetonitrile + 1,1,2,2-Tetrachloroethane), (Phenylacetonitrile + Trichloroethene), and (Phenylacetonitrile + Tetrachloroethene) at Temperatures of (303.15, 308.15, and 313.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53354e+01
Coeff. B	-4.87262e+03
Coeff. C	-5.13390e+01
Temperature range (K), min.	375.15

Temperature range (K), max.	537.44

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. C	-1.15248e+00
Temperature range (K), min.	273.15
Temperature range (K), max.	273.15

Datasets

Viscosity, Pa*s

Temperature, K - Liquid	Pressure, kPa - Liquid	Viscosity, Pa*s - Liquid
308.15	101.30	0.0015850

Reference *https://www.doi.org/10.1021/je8003723*

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	298.15	1012.89

Reference *https://www.doi.org/10.1016/j.jct.2017.09.027*

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Volumetric and Transport Properties of Binary Liquid Mixtures of Aliphatic Ketones with Phenylacetonitrile at T = 308.15 K:	https://www.doi.org/10.1021/je8003723
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Volumetric and Transport Properties of Binary Liquid Mixtures of Phenylacetonitrile with Aliphatic Esters at (293.15 to 313.15) K: Excess Molar Volumes and Sound Speed in (Phenylacetonitrile + 1,2-Dichloroethane), (Phenylacetonitrile + 1,1,2-Trichloroethane), (Phenylacetonitrile + 1,1,2,2-Tetrachloroethane), (Phenylacetonitrile + Trichloroethene), and (Phenylacetonitrile + Tetrachloroethene) at Temperatures of (303.15, 308.15, and 313.15) K:	https://www.doi.org/10.1021/je900525f
Thermodynamics of mixtures containing aromatic nitriles.	https://www.doi.org/10.1016/j.jct.2017.09.027
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1400
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C140294&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
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
rhol:	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