Benzenepropanenitrile

Other names:	(2-cyanoethyl)benzene
	1-phenyl-2-cyanoethane
	2-Phenylethyl cyanide
	3-Phenylpropiononitrile
	3-phenylpropanenitrile
	3-phenylpropionitrile
	Benzenepropanitrile
	Benzenepropionitrile
	Hydrocinnamique nitrile
	Hydrocinnamonitrile
	NSC 16936
	Phenethyl cyanide
	Phenylpropionitrile
	«beta»-Phenyl propionitrile
	«beta»-Phenylethyl cyanide
Inchi:	InChI=1S/C9H9N/c10-8-4-7-9-5-2-1-3-6-9/h1-3,5-6H,4,7H2
InchiKey:	ACRWYXSKEHUQDB-UHFFFAOYSA-N
Formula:	C9H9N
SMILES:	N#CCCc1ccccc1
Mol. weight [g/mol]:	131.17
CAS:	645-59-0

Physical Properties

Property code	Value	Unit	Source
gf	270.49	kJ/mol	Joback Method
hf	172.32	kJ/mol	Joback Method
hfus	14.61	kJ/mol	Joback Method
hvap	48.38	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.143		Crippen Method
mcvol	115.290	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	1186.00		NIST Webbook
rinpol	1242.60		NIST Webbook
rinpol	1186.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1230.00		NIST Webbook

rinpol	1244.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1202.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1188.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1231.00		NIST Webbook
ripol	2048.00		NIST Webbook
ripol	2041.00		NIST Webbook
tb	534.20	K	NIST Webbook
tc	761.51	K	Joback Method
tf	282.60	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.12	J/mol×K	534.08	Joback Method
cpg	255.68	J/mol×K	571.99	Joback Method
cpg	266.47	J/mol×K	609.89	Joback Method
cpg	276.52	J/mol×K	647.80	Joback Method
cpg	285.87	J/mol×K	685.70	Joback Method
cpg	294.57	J/mol×K	723.61	Joback Method
cpg	302.65	J/mol×K	761.51	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.20	K	1.00	NIST Webbook

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	298.15	996.44

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C645590&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamics of mixtures containing aromatic nitriles:	https://www.doi.org/10.1016/j.jct.2017.09.027
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume