Benzonitrile, 3-methyl-

Other names:	1-Methyl-3-cyanobenzene
	3-Cyanotoluene
	3-Methylbenzonitrile
	3-Toluenkarbonitril
	3-Tolunitrile
	M-CYANOTOLUENE
	M-METHYLBENZONITRILE
	M-TOLUNITRILE
	M-TOLYNITRILE
	MTN
	NSC 75453
	Nitril kyseliny m-toluylove
	m-Toluenenitrile
	m-Toluonitrile
	m-Tolylnitrile
	meta-Tolunitrile
Inchi:	InChI=1S/C8H7N/c1-7-3-2-4-8(5-7)6-9/h2-5H,1H3
InchiKey:	BOHCMQZJWOGWTA-UHFFFAOYSA-N
Formula:	C8H7N
SMILES:	Cc1cccc(C#N)c1
Mol. weight [g/mol]:	117.15
CAS:	620-22-4

Physical Properties

Property code	Value	Unit	Source
gf	252.44	kJ/mol	Joback Method
hf	181.49	kJ/mol	Joback Method
hfus	11.63	kJ/mol	Joback Method
hvap	46.82	kJ/mol	Joback Method
ie	9.40	eV	NIST Webbook
ie	9.34	eV	NIST Webbook
ie	9.58 ± 0.05	eV	NIST Webbook
ie	9.66 ± 0.05	eV	NIST Webbook
log10ws	-2.30		Crippen Method
logp	1.867		Crippen Method
mcvol	101.200	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method

tb	487.90 ± 0.50	K	NIST Webbook
tb	487.30 ± 0.60	K	NIST Webbook
tc	749.09	K	Joback Method
tf	283.85	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.23	J/mol×K	749.09	Joback Method
cpg	245.15	J/mol×K	710.28	Joback Method
cpg	237.53	J/mol×K	671.46	Joback Method
cpg	229.35	J/mol×K	632.64	Joback Method
cpg	220.58	J/mol×K	593.82	Joback Method
cpg	211.18	J/mol×K	555.00	Joback Method
cpg	201.15	J/mol×K	516.18	Joback Method
hvapt	50.80	kJ/mol	394.00	NIST Webbook
pvap	0.03	kPa	294.30	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.03	kPa	297.20	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.04	kPa	300.00	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.05	kPa	302.10	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.02	kPa	292.40	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study

pvap	0.07	kPa	307.70	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.08	kPa	309.20	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.08	kPa	310.10	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.09	kPa	312.00	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.10	kPa	313.70	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.02	kPa	290.30	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.02	kPa	288.30	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.01	kPa	285.70	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.01	kPa	283.70	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	8.29e-03	kPa	281.30	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study

pvap	7.20e-03	kPa	279.80	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.05	kPa	304.10	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.20	K	2.70	NIST Webbook
tbrp	357.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41522e+01
Coeff. B	-3.91841e+03
Coeff. C	-7.63000e+01
Temperature range (K), min.	358.92
Temperature range (K), max.	519.52

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C620224&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study: https://www.doi.org/10.1016/j.jct.2015.07.025

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1398

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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume