Benzonitrile, 2-methyl-

Other names:	1-Cyano-2-methylbenzene
	1-Methyl-2-cyanobenzene
	2-Cyanotoluene
	2-Methylbenzenecarbonitrile
	2-Methylbenzonitrile
	2-Toluenkarbonitril
	2-Tolunitrile
	NSC 66549
	O-CYANOTOLUENE
	O-METHYLBENZONITRILE
	O-TOLUNITRILE
	O-TOLYNITRILE
	o-Toluic nitrile
	o-Toluonitrile
	o-Tolylnitrile
	o-toluenecarbonitrile
Inchi:	InChI=1S/C8H7N/c1-7-4-2-3-5-8(7)6-9/h2-5H,1H3
InchiKey:	NWPNXBQSRGKSJB-UHFFFAOYSA-N
Formula:	C8H7N
SMILES:	Cc1ccccc1C#N
Mol. weight [g/mol]:	117.15
CAS:	529-19-1

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	9.38	eV	NIST Webbook
ie	9.40	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
rinpol	172.60		NIST Webbook
rinpol	172.60		NIST Webbook

ripol	1912.00		NIST Webbook
ripol	1912.00		NIST Webbook
tb	478.20	K	NIST Webbook
tb	477.90 ± 0.60	K	NIST Webbook
tb	478.00 ± 0.50	K	NIST Webbook
tb	478.35 ± 1.00	K	NIST Webbook
tc	749.09	K	Joback Method
tf	261.10 ± 0.02	K	NIST Webbook
tf	260.90 ± 0.35	K	NIST Webbook
tf	262.75 ± 0.25	K	NIST Webbook
tf	262.53 ± 0.30	K	NIST Webbook
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.15	J/mol×K	516.18	Joback Method
cpg	211.18	J/mol×K	555.00	Joback Method
cpg	220.58	J/mol×K	593.82	Joback Method
cpg	229.35	J/mol×K	632.64	Joback Method
cpg	237.53	J/mol×K	671.46	Joback Method
cpg	245.15	J/mol×K	710.28	Joback Method
cpg	252.23	J/mol×K	749.09	Joback Method
pvap	0.05	kPa	298.10	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.02	kPa	289.20	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.03	kPa	290.30	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.03	kPa	292.40	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study

pvap	0.04	kPa	296.30	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.02	kPa	287.40	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.06	kPa	300.70	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.08	kPa	305.10	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.10	kPa	308.20	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.12	kPa	311.00	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.13	kPa	312.00	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.12	kPa	312.00	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.15	kPa	314.90	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.16	kPa	316.10	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study

pvap	0.19	kPa	318.10	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.22	kPa	321.10	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.24	kPa	322.20	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
pvap	0.27	kPa	324.20	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42131e+01
Coeff. B	-3.87747e+03
Coeff. C	-7.40760e+01
Temperature range (K), min.	352.52
Temperature range (K), max.	509.67

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1397
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C529191&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

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
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