Benzonitrile, 4-methyl-

Other names:	1-Cyano-4-methylbenzene
	1-Methyl-4-cyanobenzene
	4-Cyanotoluene
	4-Methylbenzonitrile
	4-Methylcyanobenzene
	4-Toluenkarbonitril
	4-Tolunitrile
	NSC 70985
	Nitril kyseliny p-toluylove
	P-CYANOTOLUENE
	P-METHYLBENZONITRILE
	P-TOLUNITRILE
	P-TOLYNITRILE
	p-Toluenenitrile
	p-Toluic nitrile
	p-Tolunitril
	p-Toluonitrile
	p-Tolylnitrile
Inchi:	InChI=1S/C8H7N/c1-7-2-4-8(6-9)5-3-7/h2-5H,1H3
InchiKey:	VCZNNAKNUVJVGX-UHFFFAOYSA-N
Formula:	C8H7N
SMILES:	Cc1ccc(C#N)cc1
Mol. weight [g/mol]:	117.15
CAS:	104-85-8

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	9.56 ± 0.05	eV	NIST Webbook
ie	9.31	eV	NIST Webbook
ie	9.33	eV	NIST Webbook
ie	9.32	eV	NIST Webbook
ie	9.76	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	1072.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	177.80		NIST Webbook
rinpol	178.10		NIST Webbook
ripol	1928.00		NIST Webbook
tb	491.30 ± 0.60	K	NIST Webbook
tb	491.30 ± 0.50	K	NIST Webbook
tb	490.75 ± 1.00	K	NIST Webbook
tb	490.80	K	NIST Webbook
tb	490.20	K	KDB
tc	723.00	K	KDB
tf	301.55 ± 0.50	K	NIST Webbook
tf	299.70 ± 1.00	K	NIST Webbook
tf	299.30	K	Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study
tf	302.60	K	KDB
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
hvapt	48.00	kJ/mol	403.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	377.70	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42002e+01
Coeff. B	-3.96104e+03
Coeff. C	-7.74120e+01
Temperature range (K), min.	362.12
Temperature range (K), max.	523.04

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1399
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104858&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

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
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

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