N-Methyl-o-toluidine

Other names:	2,N-Dimethylaniline
	Benzenamine, N,2-dimethyl-
	N,2-Dimethylaniline
	N,2-Dimethylbenzenamine
	o-Toluidine, N-methyl-
Inchi:	InChI=1S/C8H11N/c1-7-5-3-4-6-8(7)9-2/h3-6,9H,1-2H3
InchiKey:	GUAWMXYQZKVRCW-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CNc1ccccc1C
Mol. weight [g/mol]:	121.18
CAS:	611-21-2

Physical Properties

Property code	Value	Unit	Source
gf	208.65	kJ/mol	Joback Method
hf	70.08	kJ/mol	Joback Method
hfus	15.23	kJ/mol	Joback Method
hvap	42.78	kJ/mol	Joback Method
ie	7.60 ± 0.10	eV	NIST Webbook
ie	7.27	eV	NIST Webbook
log10ws	-1.96		Crippen Method
logp	2.037		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	480.70	K	NIST Webbook
tc	678.02	K	Joback Method
tf	271.52	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.64	J/mol×K	464.27	Joback Method
cpg	231.43	J/mol×K	499.89	Joback Method

cpg	243.51	J/mol×K	535.52	Joback Method
cpg	254.89	J/mol×K	571.14	Joback Method
cpg	265.62	J/mol×K	606.77	Joback Method
cpg	275.70	J/mol×K	642.39	Joback Method
cpg	285.18	J/mol×K	678.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.20	K	2.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47947e+01
Coeff. B	-4.13089e+03
Coeff. C	-7.47710e+01
Temperature range (K), min.	359.52
Temperature range (K), max.	510.37

Sources

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
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C611212&Units=SI

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