

N-METHYL-M-TOLUIDINE

Other names:	Aniline, N,m-dimethyl- N,3-Dimethylaniline N,3-Dimethylbenzenamine N-Methyl-3-methylaniline m,N-Dimethylaniline m-Toluidine, N-methyl-
Inchi:	InChI=1S/C8H11N/c1-7-4-3-5-8(6-7)9-2/h3-6,9H,1-2H3
InchiKey:	FBGJJTQNZVNEQU-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	CNc1cccc(C)c1
Mol. weight [g/mol]:	121.18
CAS:	696-44-6

Physical Properties

Property code	Value	Unit	Source
af	0.4351		Cheméo Relay (1.0)
gf	208.65	kJ/mol	Joback Method
hf	61.18	kJ/mol	Cheméo Relay (1.0)
hfus	15.23	kJ/mol	Joback Method
hvap	58.07	kJ/mol	Cheméo Relay (1.0)
ie	7.26	eV	NIST Webbook
ie	7.50 ± 0.10	eV	NIST Webbook
log10ws	-1.76		Cheméo Relay (1.0)
logp	2.037		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
ripol	1811.40		NIST Webbook
ripol	1810.70		NIST Webbook
tb	479.70	K	NIST Webbook
tc	717.88	K	Cheméo Relay (1.0)
tf	239.02	K	Cheméo Relay (1.0)
vc	0.393	m3/kmol	Cheméo Relay (1.0)

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

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47928e+01
Coeff. B	-4.12279e+03
Coeff. C	-7.44930e+01
Temperature range (K), min.	358.72
Temperature range (K), max.	509.32

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C696446&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

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

Legend

af:	Acentric Factor
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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