

1,2-Benzenediamine, 3-methyl-

Other names:	Toluene-2,3-diamine 2,3-Diaminotoluene 2,3-Toluylenediamine 2,3-Tolylenediamine
Inchi:	InChI=1S/C7H10N2/c1-5-3-2-4-6(8)7(5)9/h2-4H,8-9H2,1H3
InchiKey:	AXNUJYHFQHQZBE-UHFFFAOYSA-N
Formula:	C7H10N2
SMILES:	Cc1cccc(N)c1N
Mol. weight [g/mol]:	122.17
CAS:	2687-25-4

Physical Properties

Property code	Value	Unit	Source
gf	234.11	kJ/mol	Joback Method
hf	93.36	kJ/mol	Joback Method
hfus	17.54	kJ/mol	Joback Method
hvap	56.06	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.159		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4596.38	kPa	Joback Method
tb	541.26	K	Joback Method
tc	781.39	K	Joback Method
tf	386.63	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.29	J/molxK	541.26	Joback Method
cpg	248.42	J/molxK	581.28	Joback Method
cpg	258.84	J/molxK	621.30	Joback Method
cpg	268.59	J/molxK	661.32	Joback Method
cpg	277.69	J/molxK	701.34	Joback Method

cpg	286.17	J/mol×K	741.37	Joback Method
cpg	294.05	J/mol×K	781.39	Joback Method

Sources

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=C2687254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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