3-Chloro-N,N-dimethylaniline

Other names: Benzenamine, 3-chloro-N,N-dimethyl-
m-Chloro-N,N-dimethylaniline
Inchi: InChI=1S/C8H10ClN/c1-10(2)8-5-3-4-7(9)6-8/h3-6H,1-2H3
InchiKey: CHHCCYVOJBBCIY-UHFFFAOYSA-N
Formula: C8H10ClN
SMILES: CN(C)c1cccc(Cl)c1
Mol. weight [g/mol]: 155.62
CAS: 6848-13-1

Physical Properties

Property code	Value	Unit	Source
gf	218.11	kJ/mol	Joback Method
hf	68.40	kJ/mol	Joback Method
hfus	17.35	kJ/mol	Joback Method
hvap	42.77	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.406		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	1271.90		NIST Webbook
rinpol	1271.90		NIST Webbook
tb	504.50 ± 0.50	K	NIST Webbook
tc	679.10	K	Joback Method
tf	281.25	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.64	J/mol×K	463.97	Joback Method
cpg	245.45	J/mol×K	499.82	Joback Method
cpg	257.46	J/mol×K	535.68	Joback Method
cpg	268.70	J/mol×K	571.53	Joback Method
cpg	279.22	J/mol×K	607.39	Joback Method

cpg	289.03	J/mol×K	643.24	Joback Method
cpg	298.20	J/mol×K	679.10	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=C6848131&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume