3-Chlorodiphenylamine

Other names: Benzenamine, 3-chloro-N-phenyl-
Diphenylamine, 3-chloro-
Inchi: InChI=1S/C12H10ClN/c13-10-5-4-8-12(9-10)14-11-6-2-1-3-7-11/h1-9,14H
InchiKey: OHHIBZKYXJDQEU-UHFFFAOYSA-N
Formula: C12H10ClN
SMILES: Clc1cccc(Nc2ccccc2)c1
Mol. weight [g/mol]: 203.67
CAS: 101-17-7

Physical Properties

Property code	Value	Unit	Source
gf	342.81	kJ/mol	Joback Method
hf	208.31	kJ/mol	Joback Method
hfus	23.82	kJ/mol	Joback Method
hvap	58.34	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	4.084		Crippen Method
mcvol	154.640	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpol	1789.60		NIST Webbook
rinpol	1789.60		NIST Webbook
tb	619.90	K	Joback Method
tc	872.29	K	Joback Method
tf	372.94	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.71	J/mol×K	619.90	Joback Method
cpg	365.98	J/mol×K	661.96	Joback Method
cpg	379.03	J/mol×K	704.03	Joback Method
cpg	390.96	J/mol×K	746.09	Joback Method
cpg	401.84	J/mol×K	788.16	Joback Method

cpg	411.75	J/mol×K	830.22	Joback Method
cpg	420.77	J/mol×K	872.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	608.70	K	96.50	NIST Webbook

Sources

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=C101177&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
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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