1-(M-CHLOROPHENYL)PIPERAZINE

Other names:	Piperazine, 1-(3-chlorophenyl)- CPP 1-(m-chlorophenyl)piperazine
Inchi:	InChI=1S/C10H13ClN2/c11-9-2-1-3-10(8-9)13-6-4-12-5-7-13/h1-3,8,12H,4-7H2
InchiKey:	VHFVKMTVMIZMIK-UHFFFAOYSA-N
Formula:	C10H13ClN2
SMILES:	Clc1cccc(N2CCNCC2)c1
Mol. weight [g/mol]:	196.68

Physical Properties

Property code	Value	Unit	Source
hf	117.61	kJ/mol	Cheméo Relay (1.0)
hvap	84.11	kJ/mol	Cheméo Relay (1.0)
ie	8.34	eV	Cheméo Relay (1.0)
log10ws	-1.41		Cheméo Relay (1.0)
logp	1.750		Crippen Method
mcvol	149.340	ml/mol	McGowan Method
rinpol	1777.10		NIST Webbook
rinpol	1777.10		NIST Webbook
tb	589.74	K	Cheméo Relay (1.0)
tf	322.23	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6640240&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point