

3-Chloro-4-methylphenyl isothiocyanate

Inchi:	InChI=1S/C8H6CINS/c1-6-2-3-7(10-5-11)4-8(6)9/h2-4H,1H3
InchiKey:	PQLHTYDGCDDPNU-UHFFFAOYSA-N
Formula:	C8H6CINS
SMILES:	<chem>Cc1ccc(N=C=S)cc1Cl</chem>
Mol. weight [g/mol]:	183.66

Physical Properties

Property code	Value	Unit	Source
hf	185.39	kJ/mol	Cheméo Relay (1.0)
ie	8.42	eV	Cheméo Relay (1.0)
logp	3.383		Crippen Method
mcvol	129.790	ml/mol	McGowan Method
tb	498.20	K	Cheméo Relay (1.0)

Sources

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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19241373&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

Latest version available from:

<https://www.chemeo.com/cid/49-724-4/3-Chloro-4-methylphenyl-isothiocyanate.pdf>

Generated by Cheméo on 2026-07-21 22:23:10.908922074 +0000 UTC m=+183686.750807482.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.