3-Chloro-4-methylphenyl isothiocyanate

Inchi: InChI=1S/C8H6ClNS/c1-6-2-3-7(10-5-11)4-8(6)9/h2-4H,1H3
InchiKey: PQLHTYDGCDDPNU-UHFFFAOYSA-N
Formula: C8H6ClNS
SMILES: Cc1ccc(N=C=S)cc1Cl
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.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=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