3,4-Dimethylphenyl isothiocyanate

Inchi: InChI=1S/C9H9NS/c1-7-3-4-9(10-6-11)5-8(7)2/h3-5H,1-2H3
InchiKey: JFSHJWKBNJMGOK-UHFFFAOYSA-N
Formula: C9H9NS
SMILES: Cc1ccc(N=C=S)cc1C
Mol. weight [g/mol]: 163.25

Physical Properties

Property code	Value	Unit	Source
hf	210.38	kJ/mol	Cheméo Relay (1.0)
ie	8.10	eV	Cheméo Relay (1.0)
logp	3.038		Crippen Method
mcvol	131.640	ml/mol	McGowan Method
tb	490.18	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19241179&Units=SI
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):

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