

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:	<chem>Cc1ccc(N=C=S)cc1C</chem>
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

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