2,6-Difluorophenyl isothiocyanate

Other names: 2,6-Difluorophenyl isothiocyanate
Inchi: InChI=1S/C7H3F2NS/c8-5-2-1-3-6(9)7(5)10-4-11/h1-3H
InchiKey: DBSXNGIBAKYMSS-UHFFFAOYSA-N
Formula: C7H3F2NS
SMILES: Fc1cccc(F)c1N=C=S
Mol. weight [g/mol]: 171.17

Physical Properties

Property code	Value	Unit	Source
ie	8.95	eV	Cheméo Relay (1.0)
logp	2.699		Crippen Method
mcvol	107.000	ml/mol	McGowan Method
tb	408.99	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=C65295694&Units=SI

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature