

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.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=C65295694&Units=SI

Legend

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

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