3-nitrothiophene

Inchi: InChI=1S/C4H3NO2S/c6-5(7)4-1-2-8-3-4/h1-3H
InchiKey: SIPCFXFCVTUAID-UHFFFAOYSA-N
Formula: C4H3NO2S
SMILES: O=[N+]([O-])c1ccsc1
Mol. weight [g/mol]: 129.14
CAS: 822-84-4

Physical Properties

Property code	Value	Unit	Source
ie	9.62	eV	NIST Webbook
ie	9.78	eV	NIST Webbook
log10ws	-1.88		Crippen Method
logp	1.656		Crippen Method
mcvol	81.530	ml/mol	McGowan Method
tb	498.20	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.20	K	1.60	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C822844&Units=SI&Mask=3FFF

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure