Thiophene, 2-nitro-

Other names: 2-Nitrothiofene
2-Nitrothiophene
Inchi: InChI=1S/C4H3NO2S/c6-5(7)4-2-1-3-8-4/h1-3H
InchiKey: JIZRGGUCOQKGQD-UHFFFAOYSA-N
Formula: C4H3NO2S
SMILES: O=[N+]([O-])c1cccs1
Mol. weight [g/mol]: 129.14
CAS: 609-40-5

Physical Properties

Property code	Value	Unit	Source
ie	9.57	eV	NIST Webbook
ie	9.77 ± 0.05	eV	NIST Webbook
ie	9.77	eV	NIST Webbook
ie	9.71	eV	NIST Webbook
ie	9.73 ± 0.05	eV	NIST Webbook
log10ws	-1.88		Crippen Method
logp	1.656		Crippen Method
mcvol	81.530	ml/mol	McGowan Method
tb	497.70	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	48.60	kJ/mol	410.50	NIST Webbook
hvapt	50.40	kJ/mol	409.50	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.77668e+01
Coeff. B	-6.82769e+03
Coeff. C	2.16250e+01
Temperature range (K), min.	368.99
Temperature range (K), max.	526.55

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C609405&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

Legend

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature