2-NITROFURAN

Other names: Furan, 2-nitro-
Nitrofuran
5-Nitrofuran
Inchi: InChI=1S/C4H3NO3/c6-5(7)4-2-1-3-8-4/h1-3H
InchiKey: FUBFWTUFPGFHOJ-UHFFFAOYSA-N
Formula: C4H3NO3
SMILES: O=[N+]([O-])c1ccco1
Mol. weight [g/mol]: 113.07

Physical Properties

Property code	Value	Unit	Source
chs	-1899.00 ± 0.40	kJ/mol	NIST Webbook
hf	-29.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-104.00 ± 0.40	kJ/mol	NIST Webbook
ie	10.04 ± 0.05	eV	NIST Webbook
ie	9.75 ± 0.05	eV	NIST Webbook
log10ws	-1.63		Cheméo Relay (1.0)
logp	1.188		Crippen Method
mcvol	71.050	ml/mol	McGowan Method
tf	296.53	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	75.00 ± 2.00	kJ/mol	277.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.20	K	1.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C609392&Units=SI
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

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation 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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point