6-NITROBENZOTHIAZOLE

Other names: Benzothiazole, 6-nitro-
Inchi: InChI=1S/C7H4N2O2S/c10-9(11)5-1-2-6-7(3-5)12-4-8-6/h1-4H
InchiKey: QLUFBCVWKTWKBF-UHFFFAOYSA-N
Formula: C7H4N2O2S
SMILES: O=[N+]([O-])c1ccc2ncsc2c1
Mol. weight [g/mol]: 180.19

Physical Properties

Property code	Value	Unit	Source
hf	171.30	kJ/mol	Cheméo Relay (1.0)
hvap	82.34	kJ/mol	Cheméo Relay (1.0)
ie	9.26	eV	Cheméo Relay (1.0)
log10ws	-3.02		Cheméo Relay (1.0)
logp	2.204		Crippen Method
mcvol	114.320	ml/mol	McGowan Method
tb	580.17	K	Cheméo Relay (1.0)
tf	434.70	K	Cheméo Relay (1.0)

Sources

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=C2942065&Units=SI

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions

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
tf:	Normal melting (fusion) point