6-NITRO-2-PHENYLINDOLIZINE

Inchi: InChI=1S/C14H10N2O2/c17-16(18)14-7-6-13-8-12(9-15(13)10-14)11-4-2-1-3-5-11/h1-10
InchiKey: MAHPGNZUNZRRFK-UHFFFAOYSA-N
Formula: C14H10N2O2
SMILES: O=[N+]([O-])c1ccc2cc(-c3ccccc3)cn2c1
Mol. weight [g/mol]: 238.25

Physical Properties

Property code	Value	Unit	Source
hf	269.09	kJ/mol	Cheméo Relay (1.0)
hvap	108.77	kJ/mol	Cheméo Relay (1.0)
ie	7.79	eV	Cheméo Relay (1.0)
log10ws	-4.88		Cheméo Relay (1.0)
logp	3.514		Crippen Method
mcvol	172.840	ml/mol	McGowan Method
tb	672.34	K	Cheméo Relay (1.0)
tf	459.96	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60891761&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

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