

1H-Isoindole-1,3(2H)-dione, 2-phenyl-

Other names:	Phthalimide, N-phenyl- Phthalanil N-Phenylphthalic acid imide N-phenylphthalimide
Inchi:	InChI=1S/C14H9NO2/c16-13-11-8-4-5-9-12(11)14(17)15(13)10-6-2-1-3-7-10/h1-9H
InchiKey:	MFUPLJQNEXUUDW-UHFFFAOYSA-N
Formula:	C14H9NO2
SMILES:	O=C1c2ccccc2C(=O)N1c1ccccc1
Mol. weight [g/mol]:	223.23
CAS:	520-03-6

Physical Properties

Property code	Value	Unit	Source
ea	1.15 ± 0.09	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
log10ws	-3.56		Crippen Method
logp	2.487		Crippen Method
mcvol	162.860	ml/mol	McGowan Method
ss	273.00	J/mol×K	NIST Webbook
tf	490.40 ± 1.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	245.90	J/mol×K	300.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cps:	Solid phase heat capacity
ea:	Electron affinity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ss:	Solid phase molar entropy at standard conditions
tf:	Normal melting (fusion) point

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