Phthalimide

Other names:	1,2-Benzenedicarboximide
	1,3-Dihydro-2H-isoindole-1,3-dione
	1,3-Isoindoledione
	1,3-Isoindolinedione
	1H-Isoindole-1,3(2H)-dione
	2-Diazoindan-1,3-dione
	Benzoimide
	Ftalimmide
	Isoindol-1,3-dione: Folpet metabolite
	Isoindole-1,3-dione
	NSC 3108
	Phenylimide
	Phthalic dicarboximide
	Phthalimid
	o-Phthalic imide
Inchi:	InChI=1S/C8H5NO2/c10-7-5-3-1-2-4-6(5)8(11)9-7/h1-4H,(H,9,10,11)
InchiKey:	XKJCHHZQLQNZHY-UHFFFAOYSA-N
Formula:	C8H5NO2
SMILES:	O=C1NC(=O)c2ccccc21
Mol. weight [g/mol]:	147.13
CAS:	85-41-6

Physical Properties

Property code	Value	Unit	Source
ea	1.01 ± 0.09	eV	NIST Webbook
gf	30.25	kJ/mol	Joback Method
hf	-127.84	kJ/mol	Joback Method
hfus	15.80	kJ/mol	Joback Method
hsub	106.30 ± 1.30	kJ/mol	NIST Webbook
hvap	51.81	kJ/mol	Joback Method
ie	9.90	eV	NIST Webbook
ie	9.78 ± 0.05	eV	NIST Webbook
log10ws	-2.61		Estimated Solubility Method
log10ws	-2.61		Aqueous Solubility Prediction Method
logp	0.570		Crippen Method

mcvol	102.080	ml/mol	McGowan Method
pc	5015.69	kPa	Joback Method
rinpol	251.70		NIST Webbook
tb	609.70	K	Joback Method
tc	879.30	K	Joback Method
tf	511.15 ± 1.00	K	NIST Webbook
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.56	J/mol×K	744.50	Joback Method
cpg	280.12	J/mol×K	789.43	Joback Method
cpg	288.83	J/mol×K	834.36	Joback Method
cpg	236.95	J/mol×K	609.70	Joback Method
cpg	248.95	J/mol×K	654.63	Joback Method
cpg	260.16	J/mol×K	699.57	Joback Method
cpg	296.64	J/mol×K	879.30	Joback Method
hfust	28.60	kJ/mol	507.20	NIST Webbook
hsubt	104.00 ± 0.40	kJ/mol	356.00	NIST Webbook
hsubt	82.80	kJ/mol	398.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85416&Units=SI

Solubility modelling and thermodynamic dissolution functions of phthalimide in ten organic solvents: https://www.doi.org/10.1016/j.jct.2015.10.024

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Solubility determination and modelling for phthalimide in mixed solvents of (acetone, ethyl acetate or acetonitrile + methanol) from (278.15 to 313.15) K: https://www.doi.org/10.1016/j.jct.2016.11.023

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Research on Dissolution Capability of Several Antofloxacin Salts: https://www.doi.org/10.1021/acs.jced.8b00288

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume