

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

Other names:	Phthalimide, N-methyl- N-Methylphthalimide Methylphthalimide
Inchi:	InChI=1S/C9H7NO2/c1-10-8(11)6-4-2-3-5-7(6)9(10)12/h2-5H,1H3
InchiKey:	ZXLYYQUMYFHCLQ-UHFFFAOYSA-N
Formula:	C9H7NO2
SMILES:	CN1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	161.16
CAS:	550-44-7

Physical Properties

Property code	Value	Unit	Source
chs	-4217.00 ± 1.80	kJ/mol	NIST Webbook
hf	-233.90 ± 2.20	kJ/mol	NIST Webbook
hfs	-325.00 ± 2.10	kJ/mol	NIST Webbook
hsub	91.10 ± 0.50	kJ/mol	NIST Webbook
hsub	91.10 ± 0.50	kJ/mol	NIST Webbook
ie	9.55 ± 0.05	eV	NIST Webbook
log10ws	-1.83		Crippen Method
logp	0.912		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
rinpol	1425.00		NIST Webbook
rinpol	1425.00		NIST Webbook
tb	559.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	91.10 ± 0.50	kJ/mol	307.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C550447&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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