

1H-Isoindole-1,3(2H)-dione, 4-nitro-

Other names:	Phthalimide, 3-nitro- 3-Nitrophthalimide
Inchi:	InChI=1S/C8H4N2O4/c11-7-4-2-1-3-5(10(13)14)6(4)8(12)9-7/h1-3H,(H,9,11,12)
InchiKey:	BONIIQYTWOPUQI-UHFFFAOYSA-N
Formula:	C8H4N2O4
SMILES:	O=C1NC(=O)c2c1cccc2[N+](=O)[O-]
Mol. weight [g/mol]:	192.13
CAS:	603-62-3

Physical Properties

Property code	Value	Unit	Source
gf	56.17	kJ/mol	Joback Method
hf	-150.07	kJ/mol	Joback Method
hfus	26.77	kJ/mol	Joback Method
hvap	69.07	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	0.478		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
tb	766.52	K	Joback Method
tc	1055.95	K	Joback Method
tf	638.64	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.73	J/molxK	766.52	Joback Method
cpg	327.10	J/molxK	814.76	Joback Method
cpg	336.36	J/molxK	863.00	Joback Method
cpg	344.47	J/molxK	911.24	Joback Method
cpg	351.38	J/molxK	959.47	Joback Method
cpg	357.07	J/molxK	1007.71	Joback Method
cpg	361.49	J/molxK	1055.95	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C603623&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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