

3-Nitro-1,8-naphthalic anhydride

Other names:	Naphthalic anhydride, 3-nitro-1H,3H-Naphtho(1,8-cd)pyran-1,3-dione, 5-nitro-3-Nitronaphthalic anhydride
Inchi:	InChI=1S/C12H5NO5/c14-11-8-3-1-2-6-4-7(13(16)17)5-9(10(6)8)12(15)18-11/h1-5H
InchiKey:	FLFLZYYDLIKGJQ-UHFFFAOYSA-N
Formula:	C12H5NO5
SMILES:	O=C1OC(=O)c2cc([N+](=O)[O-])cc3cccc1c23
Mol. weight [g/mol]:	243.17
CAS:	3027-38-1

Physical Properties

Property code	Value	Unit	Source
gf	13.04	kJ/mol	Joback Method
hf	-222.84	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	78.03	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	2.059		Crippen Method
mcvol	152.290	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	860.40	K	Joback Method
tc	1148.18	K	Joback Method
tf	650.48	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.32	J/molxK	860.40	Joback Method
cpg	441.22	J/molxK	908.36	Joback Method
cpg	450.00	J/molxK	956.33	Joback Method
cpg	457.73	J/molxK	1004.29	Joback Method
cpg	464.45	J/molxK	1052.25	Joback Method
cpg	470.22	J/molxK	1100.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3027381&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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