

1,2-Naphthalenedione, 1-(phenylhydrazone)

Inchi:	InChI=1S/C16H12N2O/c19-15-11-10-12-6-4-5-9-14(12)16(15)18-17-13-7-2-1-3-8-13/h1-
InchiKey:	ZONYAPYTDIVJGG-VLGSPTGOSA-N
Formula:	C16H12N2O
SMILES:	O=C1C=Cc2ccccc2C1=NNc1ccccc1
Mol. weight [g/mol]:	248.28
CAS:	1602-30-8

Physical Properties

Property code	Value	Unit	Source
hf	189.58	kJ/mol	Joback Method
hvap	71.94	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.099		Crippen Method
mcvol	190.850	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
tb	835.81	K	Joback Method
tc	1109.31	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1602308&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

hf:	Enthalpy of formation 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

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