

m-Nitrobenzhydrazide

Other names:	3-Nitrobenzoic acid hydrazide m-Nitrobenzhydrazide Benzoic acid, 3-nitro-, hydrazide m-Nitrobenzoic acid hydrazide m-Nitrobenzoic hydrazide m-Nitrobenzoylhydrazide m-Nitrobenzoylhydrazine Benzoic acid, m-nitro-, hydrazide 3-Nitrobenzoylhydrazine NSC 123864 NSC 3558 3-nitrobenzohydrazide
Inchi:	InChI=1S/C7H7N3O3/c8-9-7(11)5-2-1-3-6(4-5)10(12)13/h1-4H,8H2,(H,9,11)
InchiKey:	NQEWXLVDAVTOHM-UHFFFAOYSA-N
Formula:	C7H7N3O3
SMILES:	NNC(=O)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	181.15

Physical Properties

Property code	Value	Unit	Source
hf	-4.59	kJ/mol	Cheméo Relay (1.0)
hfus	30.79	kJ/mol	Joback Method
hvap	88.82	kJ/mol	Cheméo Relay (1.0)
ie	9.56	eV	Cheméo Relay (1.0)
log10ws	-1.90		Cheméo Relay (1.0)
logp	0.198		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
tb	583.46	K	Cheméo Relay (1.0)
tf	417.74	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.71	J/mol×K	719.63	Joback Method

cpg	330.87	J/mol×K	762.82	Joback Method
cpg	339.15	J/mol×K	806.01	Joback Method
cpg	346.62	J/mol×K	849.20	Joback Method
cpg	353.32	J/mol×K	892.39	Joback Method
cpg	359.30	J/mol×K	935.58	Joback Method
cpg	364.62	J/mol×K	978.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C618940&Units=SI
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
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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