

2-Nitrobenzaldoxime

Other names:	o-Nitrobenzaldoxime syn-O-Nitrobenzaldoxime Benzaldehyde, 2-nitro-, oxime 2-nitrobenzaldehyde oxime
Inchi:	InChI=1S/C7H6N2O3/c10-8-5-6-3-1-2-4-7(6)9(11)12/h1-5,10H
InchiKey:	IHMGDCCTWRRUDX-UHFFFAOYSA-N
Formula:	C7H6N2O3
SMILES:	O=[N+]([O-])c1ccccc1C=NO
Mol. weight [g/mol]:	166.13
CAS:	6635-41-2

Physical Properties

Property code	Value	Unit	Source
hf	-43.52	kJ/mol	Joback Method
hvap	70.70	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.403		Crippen Method
mcvol	114.700	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	711.92	K	Joback Method
tc	953.51	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6635412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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