

Benzaldehyde, oxime

Other names:	Benzaldoxime
Inchi:	InChI=1S/C7H7NO/c9-8-6-7-4-2-1-3-5-7/h1-6,9H
InchiKey:	VTWKXBJHBYJBI-UHFFFAOYSA-N
Formula:	C7H7NO
SMILES:	ON=Cc1ccccc1
Mol. weight [g/mol]:	121.14
CAS:	932-90-1

Physical Properties

Property code	Value	Unit	Source
chs	-3797.00	kJ/mol	NIST Webbook
hf	-21.29	kJ/mol	Joback Method
hfs	25.00	kJ/mol	NIST Webbook
hvap	53.44	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	1.495		Crippen Method
mcvol	97.280	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	555.10	K	Joback Method
tc	773.37	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=C932901&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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