

BENZALDEHYDE, 4-HYDROXY-, OXIME

Other names:	Benzaldehyde, p-hydroxy-, oxime p-Hydroxybenzaldehyde oxime p-Hydroxybenzaldoxime 4-Hydroxybenzaldehyde oxime 4-Hydroxybenzaldoxime
Inchi:	InChI=1S/C7H7NO2/c9-7-3-1-6(2-4-7)5-8-10/h1-5,9-10H
InchiKey:	LJEARAFLOCEYHX-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	ON=Cc1ccc(O)cc1
Mol. weight [g/mol]:	137.14

Physical Properties

Property code	Value	Unit	Source
hf	-70.63	kJ/mol	Cheméo Relay (1.0)
hvap	86.19	kJ/mol	Cheméo Relay (1.0)
ie	8.35	eV	Cheméo Relay (1.0)
log10ws	-0.66		Cheméo Relay (1.0)
logp	1.200		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
tb	577.60	K	Cheméo Relay (1.0)
tf	433.71	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C699069&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/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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