

Benzaldehyde oxime

Other names:	benzaldoxime
Inchi:	InChI=1S/C7H7NO/c9-8-6-7-4-2-1-3-5-7/h1-6,9H/b8-6+
InchiKey:	VTWKXBJHBHYJBI-SOFGYWHQSA-N
Formula:	C7H7NO
SMILES:	ON=Cc1ccccc1
Mol. weight [g/mol]:	121.14

Physical Properties

Property code	Value	Unit	Source
hf	-21.29	kJ/mol	Joback Method
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
tf	302.85	K	Kinetics-based simulation approach to evaluate thermal hazards of benzaldehyde oxime by DSC tests

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Kinetics-based simulation approach to evaluate thermal hazards of benzaldehyde oxime by DSC tests:	https://www.doi.org/10.1016/j.tca.2017.07.015
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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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