

«beta»-Benzilmonoxime

Other names:	«alpha»-Benzilmonoxime Benzil monoxime Benzil, «beta»-monoxime Benzil, monooxime Ethanedione, diphenyl-, monooxime 1,2-Diphenylethanedione monoxime «alpha»-Benzil monooxime Benzil, oxime Benzil «alpha»-monoxime alpha-Benzil monoxime 2-Hydroxyimino-2-phenylacetophenone NSC 658
Inchi:	InChI=1S/C14H11NO2/c16-14(12-9-5-2-6-10-12)13(15-17)11-7-3-1-4-8-11/h1-10,17H
InchiKey:	OLBYFEGTUWWPTR-UHFFFAOYSA-N
Formula:	C14H11NO2
SMILES:	O=C(C(=NO)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	225.24
CAS:	14090-77-8

Physical Properties

Property code	Value	Unit	Source
hf	-51.61	kJ/mol	Joback Method
hvap	78.13	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.748		Crippen Method
mcvol	173.720	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
tb	795.69	K	Joback Method
tc	1037.06	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14090778&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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>

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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