BENZIL .alpha.-MONOXIME

Other names:	1,2-Diphenylethanedione monoxime
	2-Hydroxyimino-2-phenylacetophenone
	Benzil monoxime
	Benzil «alpha»-monoxime
	Benzil, monooxime
	Benzil, oxime
	Benzil, «beta»-monoxime
	Ethanedione, diphenyl-, monooxime
	NSC 658
	alpha-Benzil monoxime
	«alpha»-Benzil monooxime
	«alpha»-Benzilmonoxime
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]:	225.25

Physical Properties

Property code	Value	Unit	Source
af	0.7453		Cheméo Relay (1.0)
gf	201.83	kJ/mol	Cheméo Relay (1.0, beta)
hf	59.65	kJ/mol	Cheméo Relay (1.0)
hvap	84.66	kJ/mol	Cheméo Relay (1.0)
ie	8.53	eV	Cheméo Relay (1.0)
log10ws	-2.97		Cheméo Relay (1.0)
logp	2.748		Crippen Method
mcvol	173.720	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
tb	611.43	K	Cheméo Relay (1.0)
tc	924.87	K	Cheméo Relay (1.0)
tf	384.20	K	Cheméo Relay (1.0)
vc	0.624	m3/kmol	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14090778&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/ci990307l

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point
vc:	Critical Volume