

Ethanedione, diphenyl-,dioxime(E,Z)

Inchi:	InChI=1S/C14H12N2O2/c17-15-13(11-7-3-1-4-8-11)14(16-18)12-9-5-2-6-10-12/h1-10,17
InchiKey:	JJZONEUCDUQVGR-VCFJNTAESA-N
Formula:	C14H12N2O2
SMILES:	ON=C(C(=NO)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	240.26
CAS:	572-43-0

Physical Properties

Property code	Value	Unit	Source
chs	-7277.20 ± 7.10	kJ/mol	NIST Webbook
hf	-18.83	kJ/mol	Joback Method
hvap	91.46	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	2.743		Crippen Method
mcvol	183.700	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
tb	910.56	K	Joback Method
tc	1146.06	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C572430&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
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
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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<https://www.chemeo.com/cid/12-340-0/Ethanedione-diphenyl-dioxime-E-Z.pdf>

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