

Ethanedione, diphenyl-, dioxime, (E,E)-

Other names: (E,E)-diphenylethanedione dioxime
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-UHFFFAOYSA-N
Formula: C14H12N2O2
SMILES: ON=C(C(=NO)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 240.26
CAS: 522-34-9

Physical Properties

Property code	Value	Unit	Source
chs	-7242.10 ± 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

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C522349&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

chs: Standard solid enthalpy of combustion

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ 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

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