

Benzylideneimine,n-(2,2-diethoxyethyl)-o-hydroxy-

Inchi: InChI=1S/C13H19NO3/c1-3-16-13(17-4-2)10-14-9-11-7-5-6-8-12(11)15/h5-9,13,15H,3-4,
InchiKey: QXNBLBWJCRLMAR-ZROIWOOFSA-N
Formula: C13H19NO3
SMILES: CCOC(CN=Cc1cccc1O)OCC
Mol. weight [g/mol]: 237.29
CAS: 116632-97-4

Physical Properties

Property code	Value	Unit	Source
hf	-439.93	kJ/mol	Joback Method
hvap	67.57	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	2.210		Crippen Method
mcvol	193.560	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
tb	725.22	K	Joback Method
tc	945.87	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=C116632974&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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