

4-Ethoxy-3'-formyl-4'-benzyloxyazobenzene

Inchi: InChI=1S/C22H20N2O3/c1-2-26-21-11-8-19(9-12-21)23-24-20-10-13-22(18(14-20)15-25
InchiKey: QMIMWGVGEBXJBU-WCWDXBQESA-N
Formula: C22H20N2O3
SMILES: CCOc1ccc(N=Nc2ccc(OCc3ccccc3)c(C=O)c2)cc1
Mol. weight [g/mol]: 360.41
CAS: 87730-61-8

Physical Properties

Property code	Value	Unit	Source
chs	-11864.80	kJ/mol	NIST Webbook
hf	-125.03	kJ/mol	Joback Method
hfs	349.20	kJ/mol	NIST Webbook
hvap	91.59	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.892		Crippen Method
mcvol	278.530	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
tb	1040.44	K	Joback Method
tc	1298.19	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=C87730618&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
hfs:	Solid phase 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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