

Glycoldial, bis-O-pentafluorobenzylloxime

Other names:	Glyoxal dioxime, O,O'-bis[(pentafluorophenyl)methyl]- Glyoxal, bis-O-[(pentafluorophenyl)methyl]oxime, (E) Glyoxal, bis-PFBO
Inchi:	InChI=1S/C16H6F10N2O2/c17-7-5(8(18)12(22)15(25)11(7)21)3-29-27-1-2-28-30-4-6-9(1
InchiKey:	VNVBOBJSRGZDCW-UHFFFAOYSA-N
Formula:	C16H6F10N2O2
SMILES:	Fc1c(F)c(F)c(CON=CC=NOCc2c(F)c(F)c(F)c(F)c2F)c(F)c1F
Mol. weight [g/mol]:	448.22
CAS:	618858-54-1

Physical Properties

Property code	Value	Unit	Source
hf	-2076.31	kJ/mol	Joback Method
hvap	65.66	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	4.783		Crippen Method
mcvol	229.580	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
rinpol	1935.00		NIST Webbook
tb	859.54	K	Joback Method
tc	1055.77	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=C618858541&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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