

Propionaldehyde, (O-pentafluorobenzyl)oxime, (Z) or (E)-

Other names:	n-Propanal, o-[(pentafluorophenyl)methyl]oxime Propanal, PFBO # 2
Inchi:	InChI=1S/C10H8F5NO/c1-2-3-16-17-4-5-6(11)8(13)10(15)9(14)7(5)12/h3H,2,4H2,1H3
InchiKey:	BOPZGAUHLLBMFA-UHFFFAOYSA-N
Formula:	C10H8F5NO
SMILES:	CCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	253.17
CAS:	932710-53-7

Physical Properties

Property code	Value	Unit	Source
hf	-1101.10	kJ/mol	Joback Method
hvap	45.08	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.295		Crippen Method
mcvol	148.400	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1193.00		NIST Webbook
rinpol	1193.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1509.00		NIST Webbook
tb	575.23	K	Joback Method
tc	754.89	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=C932710537&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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