

Acetone, (O-pentafluorobenzyl)oxime

Other names:	Acetone oxime, o-[(pentafluorophenyl)methyl]- Acetone, PFBO
Inchi:	InChI=1S/C10H8F5NO/c1-4(2)16-17-3-5-6(11)8(13)10(15)9(14)7(5)12/h3H2,1-2H3
InchiKey:	DLIFNTQMBOCKTL-UHFFFAOYSA-N
Formula:	C10H8F5NO
SMILES:	CC(C)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	253.17

Physical Properties

Property code	Value	Unit	Source
hf	-1110.89	kJ/mol	Joback Method
hvap	45.16	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.295		Crippen Method
mcvol	148.400	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1167.00		NIST Webbook
rinpol	1167.00		NIST Webbook
ripol	1466.00		NIST Webbook
ripol	1466.00		NIST Webbook
tb	575.11	K	Joback Method
tc	757.56	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=U157013&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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