

n-Nonanal, o-[(pentafluorophenyl)methyl]oxime

Other names: Nonanal, O-[(pentafluorophenyl)methyl]oxime, (E)

Nonanal, PFBO # 2

Inchi: InChI=1S/C16H20F5NO/c1-2-3-4-5-6-7-8-9-22-23-10-11-12(17)14(19)16(21)15(20)13(11)

InchiKey: DYTJHXNVXCBNHN-UHFFFAOYSA-N

Formula: C16H20F5NO

SMILES: CCCCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 337.33

Physical Properties

Property code	Value	Unit	Source
hf	-1224.94	kJ/mol	Joback Method
hvap	58.44	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.635		Crippen Method
mcvol	232.940	ml/mol	McGowan Method
pc	1235.48	kPa	Joback Method
ripol	2047.00		NIST Webbook
tb	712.51	K	Joback Method
tc	888.15	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U288100&Units=SI>

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

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>

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
ri_{pol}:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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