

N-Tridecanal oxime, o-[(pentafluorophenyl)methyl]-

Other names: Tridecanal, PFBO # 1
Inchi: InChI=1S/C20H28F5NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-26-27-14-15-16(21)18(23)20(25)
InchiKey: RBTHWMFPSLXCNJ-UHFFFAOYSA-N
Formula: C20H28F5NO
SMILES: CCCCCCCCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 393.43

Physical Properties

Property code	Value	Unit	Source
hf	-1307.50	kJ/mol	Joback Method
hvap	67.34	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.196		Crippen Method
mcvol	289.300	ml/mol	McGowan Method
pc	959.10	kPa	Joback Method
ripol	2141.00		NIST Webbook
ripol	2443.00		NIST Webbook
tb	804.03	K	Joback Method
tc	986.82	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U288142&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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