

(Z)-3-Hexenal, PFBO # 1

Inchi: InChI=1S/C13H12F5NO/c1-2-3-4-5-6-19-20-7-8-9(14)11(16)13(18)12(17)10(8)15/h3-4,6
InchiKey: PLYBPQWHMHMGKM-LHBUDWCQSA-N
Formula: C13H12F5NO
SMILES: CCC=CCC=NOc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 293.23

Physical Properties

Property code	Value	Unit	Source
hf	-1045.80	kJ/mol	Joback Method
hvap	51.72	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.241		Crippen Method
mcvol	186.370	ml/mol	McGowan Method
pc	1593.62	kPa	Joback Method
ripol	1800.00		NIST Webbook
ripol	1800.00		NIST Webbook
tb	648.03	K	Joback Method
tc	829.81	K	Joback Method

Sources

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=R576122&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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<https://www.chemeo.com/cid/122-224-7/Z-3-Hexenal-PFBO-1.pdf>

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