

Hexanal, PFBO # 1

Inchi:	InChI=1S/C13H14F5NO/c1-2-3-4-5-6-19-20-7-8-9(14)11(16)13(18)12(17)10(8)15/h6H,2-
InchiKey:	GPAVMFOMYSGJDM-UHFFFAOYSA-N
Formula:	C13H14F5NO
SMILES:	CCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	295.25

Physical Properties

Property code	Value	Unit	Source
hf	-1163.02	kJ/mol	Joback Method
hvap	51.76	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.465		Crippen Method
mcvol	190.670	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	1454.00		NIST Webbook
rinpol	1456.00		NIST Webbook
ripol	1755.00		NIST Webbook
tb	643.87	K	Joback Method
tc	819.87	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R399074&Units=SI

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

Latest version available from:

<https://www.cheméo.com/cid/44-657-4/Hexanal-PFBO-1.pdf>

Generated by Cheméo on 2025-12-05 23:31:33.729132129 +0000 UTC m=+4725691.259172811.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.