

(E,E)-2,4-Heptadienal, PFBO # 1

Inchi:	InChI=1S/C14H12F5NO/c1-2-3-4-5-6-7-20-21-8-9-10(15)12(17)14(19)13(18)11(9)16/h3-
InchiKey:	GAHPKCBQENDGSH-YDJHLNIVSA-N
Formula:	C14H12F5NO
SMILES:	CCC=CC=CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	305.24

Physical Properties

Property code	Value	Unit	Source
hf	-949.22	kJ/mol	Joback Method
hvap	53.90	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.407		Crippen Method
mccvol	196.160	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
rinpol	1691.00		NIST Webbook
ripol	2153.00		NIST Webbook
tb	675.07	K	Joback Method
tc	861.61	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=R575629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/23-264-3/E-E-2-4-Heptadienal-PFBO-1.pdf>

Generated by Cheméo on 2025-12-05 16:58:15.416019701 +0000 UTC m=+4702092.946060374.

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