

Undecanal, PFBO # 1

Inchi: InChI=1S/C18H24F5NO/c1-2-3-4-5-6-7-8-9-10-11-24-25-12-13-14(19)16(21)18(23)17(22)
InchiKey: XJDXRHQPJGTNHN-UHFFFAOYSA-N
Formula: C18H24F5NO
SMILES: CCCCCCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 365.38

Physical Properties

Property code	Value	Unit	Source
hf	-1266.22	kJ/mol	Joback Method
hvap	62.89	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.415		Crippen Method
mcvol	261.120	ml/mol	McGowan Method
pc	1084.20	kPa	Joback Method
rinpol	1949.00		NIST Webbook
rinpol	1949.00		NIST Webbook
ripol	2239.00		NIST Webbook
ripol	2239.00		NIST Webbook
tb	758.27	K	Joback Method
tc	936.21	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R575961&Units=SI>

Legend

hf:	Enthalpy of formation at standard conditions
hvac:	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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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