

Decanal, PFBO # 1

Inchi: InChI=1S/C17H22F5NO/c1-2-3-4-5-6-7-8-9-10-23-24-11-12-13(18)15(20)17(22)16(21)14
InchiKey: NUGDFCWVLOJWOP-UHFFFAOYSA-N
Formula: C17H22F5NO
SMILES: CCCCCCCCC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 351.35

Physical Properties

Property code	Value	Unit	Source
hf	-1245.58	kJ/mol	Joback Method
hvap	60.66	kJ/mol	Joback Method
log10ws	-7.44		Crippen Method
logp	6.025		Crippen Method
mcvol	247.030	ml/mol	McGowan Method
pc	1156.14	kPa	Joback Method
rinpol	1849.00		NIST Webbook
ripol	2138.00		NIST Webbook
tb	735.39	K	Joback Method
tc	911.89	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R575347&Units=SI>
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>

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

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