(Z)-3-Methylhexanal, PFBO # 1

Inchi: InChI=1S/C14H14F5NO/c1-3-4-8(2)5-6-20-21-7-9-10(15)12(17)14(19)13(18)11(9)16/h4,
InchiKey: XTHCNSDNHMWGLJ-PHPVGLLJSA-N
Formula: C14H14F5NO
SMILES: CCC=C(C)CC=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 307.26

Physical Properties

Property code	Value	Unit	Source
hf	-1076.23	kJ/mol	Joback Method
hvap	54.02	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	4.631		Crippen Method
mcvol	200.460	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	1457.00		NIST Webbook
rinpol	1457.00		NIST Webbook
tb	670.79	K	Joback Method
tc	853.80	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R576142&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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