

Propyl,hexaflouro-2-triflouromethyl

Inchi: InChI=1S/C4F9/c5-1(3(8,9)10)2(6,7)4(11,12)13
InchiKey: VWIYRCOUQNNFI-UHFFFAOYSA-N
Formula: C4F9
SMILES: F[C](C(F)(F)F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 219.03
CAS: 4556-27-8

Physical Properties

Property code	Value	Unit	Source
ea	3.55 ± 0.50	eV	NIST Webbook
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log10ws	-3.10		Crippen Method
logp	3.248		Crippen Method
mcvol	81.000	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4556278&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ea: Electron affinity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/72-862-5/Propyl-hexaflouro-2-triflouromethyl.pdf>

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