1-(4-Ethylpiperazin-1-yl)-2,2,2-trifluoroethanone

Inchi: InChI=1S/C8H13F3N2O/c1-2-12-3-5-13(6-4-12)7(14)8(9,10)11/h2-6H2,1H3
InchiKey: QXUTXTAYZAVQKI-UHFFFAOYSA-N
Formula: C8H13F3N2O
SMILES: CCN1CCN(C(=O)C(F)(F)F)CC1
Mol. weight [g/mol]: 210.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.64		Crippen Method
logp	0.713		Crippen Method
mcvol	139.560	ml/mol	McGowan Method
rinpol	1231.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373192&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices