Proline, N-(trifluoroacetyl)-, methyl ester

Other names: N-trifluoroacetyl-l-proline, methyl ester
Inchi: InChI=1S/C8H10F3NO3/c1-15-6(13)5-3-2-4-12(5)7(14)8(9,10)11/h5H,2-4H2,1H3
InchiKey: SZHIHLKFIRSJER-UHFFFAOYSA-N
Formula: C8H10F3NO3
SMILES: COC(=O)C1CCCN1C(=O)C(F)(F)F
Mol. weight [g/mol]: 225.17
CAS: 715-58-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.05		Crippen Method
logp	0.713		Crippen Method
mcvol	137.020	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	57.90	kJ/mol	413.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C715582&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume