

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

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