

# Trifluoroacetylurea

**Inchi:** InChI=1S/C3H3F3N2O2/c4-3(5,6)1(9)8-2(7)10/h(H3,7,8,9,10)  
**InchiKey:** XQXVUQWCFHYDNA-UHFFFAOYSA-N  
**Formula:** C3H3F3N2O2  
**SMILES:** N=C(O)N=C(O)C(F)(F)F  
**Mol. weight [g/mol]:** 156.06  
**CAS:** 760-41-8

## Physical Properties

Property code	Value	Unit	Source
hf	-736.03	kJ/mol	Joback Method
hvap	67.36	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	0.998		Crippen Method
mcvol	81.540	ml/mol	McGowan Method
tb	607.88	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C760418&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/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

**tb:** Normal Boiling Point Temperature

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