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
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