L-Homoserine lactone, N-trifluoroacetyl-

Inchi: InChI=1S/C6H6F3NO3/c7-6(8,9)5(12)10-3-1-2-13-4(3)11/h3H,1-2H2,(H,10,12)
InchiKey: GYQJCHTYZDUOOF-UHFFFAOYSA-N
Formula: C6H6F3NO3
SMILES: O=C1OCCC1N=C(O)C(F)(F)F
Mol. weight [g/mol]: 197.11

Physical Properties

Property code	Value	Unit	Source
hf	-1053.27	kJ/mol	Joback Method
hvap	54.29	kJ/mol	Joback Method
log10ws	-0.85		Crippen Method
logp	0.821		Crippen Method
mcvol	108.840	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
rinpol	1183.00		NIST Webbook
rinpol	1183.00		NIST Webbook
tb	610.05	K	Joback Method
tc	814.71	K	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374761&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature