

L-(+)-Threose, tris(trifluoroacetate), methyloxime (syn)

Inchi:	InChI=1S/C11H8F9NO7/c1-25-21-2-4(27-7(23)10(15,16)17)5(28-8(24)11(18,19)20)3-26
InchiKey:	LXLUTTKJBAJCOL-UHFFFAOYSA-N
Formula:	C11H8F9NO7
SMILES:	CON=CC(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)OC(=O)C(F)(F)F
Mol. weight [g/mol]:	437.17

Physical Properties

Property code	Value	Unit	Source
hf	-2856.57	kJ/mol	Joback Method
hvap	61.26	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.672		Crippen Method
mcvol	215.650	ml/mol	McGowan Method
pc	1490.74	kPa	Joback Method
rinpol	1075.10		NIST Webbook
rinpol	1075.10		NIST Webbook
tb	761.91	K	Joback Method
tc	939.63	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380242&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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