L-(+)-Threose, tris(trifluoroacetate) (isomer 3)

Inchi: InChI=1S/C10H5F9O7/c11-8(12,13)5(20)24-2-1-23-4(26-7(22)10(17,18)19)3(2)25-6(21)9
InchiKey: RKEXFFCZGAODQO-UHFFFAOYSA-N
Formula: C10H5F9O7
SMILES: O=C(OC1COC(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 408.13

Physical Properties

Property code	Value	Unit	Source
gf	-2478.20	kJ/mol	Joback Method
hf	-2887.57	kJ/mol	Joback Method
hfus	39.55	kJ/mol	Joback Method
hvap	58.23	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.396		Crippen Method
mcvol	185.020	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	1006.60		NIST Webbook
tb	673.70	K	Joback Method
tc	845.58	K	Joback Method
tf	460.50	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.84	J/mol×K	673.70	Joback Method
cpg	574.31	J/mol×K	702.35	Joback Method
cpg	584.03	J/mol×K	730.99	Joback Method
cpg	592.99	J/mol×K	759.64	Joback Method
cpg	601.24	J/mol×K	788.29	Joback Method
cpg	608.79	J/mol×K	816.94	Joback Method
cpg	615.66	J/mol×K	845.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380220&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

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume