2-Deoxy-D-ribofuranose, tris(trifluoroacetate) (isomer 1)

Inchi: InChI=1S/C11H7F9O7/c12-9(13,14)6(21)24-2-4-3(26-7(22)10(15,16)17)1-5(25-4)27-8(23

InchiKey: YVUVKBYPZNQSLH-UHFFFAOYSA-N

Formula: C11H7F9O7

SMILES: O=C(OCC1OC(OC(=O)C(F)(F)F)CC1OC(=O)C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 422.15

Physical Properties

Property code	Value	Unit	Source
gf	-2469.78	kJ/mol	Joback Method
hf	-2908.21	kJ/mol	Joback Method
hfus	42.14	kJ/mol	Joback Method
hvap	60.46	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.786		Crippen Method
mcvol	199.110	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	1164.60		NIST Webbook
rinpol	1164.60		NIST Webbook
tb	696.58	K	Joback Method
tc	868.85	K	Joback Method
tf	471.77	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.16	J/mol×K	696.58	Joback Method
cpg	626.07	J/mol×K	725.29	Joback Method
cpg	636.18	J/mol×K	754.00	Joback Method
cpg	645.52	J/mol×K	782.72	Joback Method
cpg	654.11	J/mol×K	811.43	Joback Method
cpg	661.97	J/mol×K	840.14	Joback Method
cpg	669.13	J/mol×K	868.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380318&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