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

Inchi: InChI=1S/C11H7F9O7/c12-9(13,14)6(21)25-3-1-5(27-8(23)11(18,19)20)24-2-4(3)26-7(22

InchiKey: RHUZEBNZNRQOPD-UHFFFAOYSA-N

Formula: C11H7F9O7

SMILES: O=C(OC1CC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)CO1)C(F)(F)F

Mol. weight [g/mol]: 422.15

Physical Properties

Property code	Value	Unit	Source
gf	-2481.88	kJ/mol	Joback Method
hf	-2914.37	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	60.63	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.786		Crippen Method
mcvol	199.110	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	1110.50		NIST Webbook
tb	700.85	K	Joback Method
tc	876.65	K	Joback Method
tf	468.25	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.48	J/mol×K	700.85	Joback Method
cpg	628.80	J/mol×K	730.15	Joback Method
cpg	639.26	J/mol×K	759.45	Joback Method
cpg	648.89	J/mol×K	788.75	Joback Method
cpg	657.69	J/mol×K	818.05	Joback Method
cpg	665.70	J/mol×K	847.35	Joback Method
cpg	672.93	J/mol×K	876.65	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=U380317&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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