1,6-Anhydro-2,3-O-isopropylidene-«beta»-D-mann trifluoroacetate

InchI: InChI=1S/C11H13F3O6/c1-10(2)19-6-5(18-9(15)11(12,13)14)4-3-16-8(17-4)7(6)20-10/h4
InchiKey: UVHBEMIQJSSZLB-UHFFFAOYSA-N
Formula: C11H13F3O6
SMILES: CC1(C)OC2C3OCC(O3)C(OC(=O)C(F)(F)F)C2O1
Mol. weight [g/mol]: 298.21

Physical Properties

Property code	Value	Unit	Source
gf	-988.82	kJ/mol	Joback Method
hf	-1479.95	kJ/mol	Joback Method
hfus	47.89	kJ/mol	Joback Method
hvap	61.53	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	0.736		Crippen Method
mcvol	169.500	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1343.60		NIST Webbook
rinpol	1343.60		NIST Webbook
tb	644.74	K	Joback Method
tc	852.01	K	Joback Method
tf	454.32	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.14	J/mol×K	644.74	Joback Method
cpg	549.55	J/mol×K	679.28	Joback Method
cpg	563.99	J/mol×K	713.83	Joback Method
cpg	577.62	J/mol×K	748.37	Joback Method
cpg	590.57	J/mol×K	782.92	Joback Method
cpg	602.98	J/mol×K	817.46	Joback Method
cpg	614.99	J/mol×K	852.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380068&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

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