1,4-Dioxane-2,3-diol, bis(trifluoroacetate)

Inchi: InChI=1S/C8H6F6O6/c9-7(10,11)5(15)19-3-4(18-2-1-17-3)20-6(16)8(12,13)14/h3-4H,1-2
InchiKey: JBPHKIBSIUKYSZ-UHFFFAOYSA-N
Formula: C8H6F6O6
SMILES: O=C(OC1OCCOC1OC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 312.12

Physical Properties

Property code	Value	Unit	Source
gf	-1770.04	kJ/mol	Joback Method
hf	-2122.23	kJ/mol	Joback Method
hfus	34.57	kJ/mol	Joback Method
hvap	53.36	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	0.896		Crippen Method
mcvol	149.960	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
tb	592.96	K	Joback Method
tc	775.71	K	Joback Method
tf	388.90	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.25	J/mol×K	592.96	Joback Method
cpg	436.89	J/mol×K	623.42	Joback Method
cpg	447.76	J/mol×K	653.88	Joback Method
cpg	457.90	J/mol×K	684.33	Joback Method
cpg	467.31	J/mol×K	714.79	Joback Method
cpg	476.00	J/mol×K	745.25	Joback Method
cpg	484.01	J/mol×K	775.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375755&Units=SI

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