1,4:3,6-dianhydro-5-deoxy-2-O-(trifluoroacetyl)-D-

Inchi: InChI=1S/C8H7F3O4/c9-8(10,11)7(12)15-5-3-14-4-1-2-13-6(4)5/h1-2,4-6H,3H2
InchiKey: FLRHIPSTQQZNJR-UHFFFAOYSA-N
Formula: C8H7F3O4
SMILES: O=C(OC1COC2C=COC21)C(F)(F)F
Mol. weight [g/mol]: 224.13

Physical Properties

Property code	Value	Unit	Source
gf	-851.72	kJ/mol	Joback Method
hf	-1143.61	kJ/mol	Joback Method
hfus	31.41	kJ/mol	Joback Method
hvap	47.98	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	0.772		Crippen Method
mcvol	122.050	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
tb	523.72	K	Joback Method
tc	723.65	K	Joback Method
tf	334.77	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.96	J/mol×K	523.72	Joback Method
cpg	334.06	J/mol×K	557.04	Joback Method
cpg	346.26	J/mol×K	590.36	Joback Method
cpg	357.59	J/mol×K	623.68	Joback Method
cpg	368.11	J/mol×K	657.01	Joback Method
cpg	377.85	J/mol×K	690.33	Joback Method
cpg	386.87	J/mol×K	723.65	Joback Method

Sources

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=U375752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume