1,6-Anhydro-«beta»-D-glucose, tris(trifluoroacetate)

Inchi: InChI=1S/C12H7F9O8/c13-10(14,15)7(22)27-3-2-1-25-6(26-2)5(29-9(24)12(19,20)21)4(3

InchiKey: HZWRZZOGPUMZBK-UHFFFAOYSA-N

Formula: C12H7F9O8

SMILES: O=C(OC1C2COC(O2)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 450.16

Physical Properties

Property code	Value	Unit	Source
gf	-2494.44	kJ/mol	Joback Method
hf	-3008.39	kJ/mol	Joback Method
hfus	51.92	kJ/mol	Joback Method
hvap	66.80	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.164		Crippen Method
mcvol	208.210	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	1179.20		NIST Webbook
rinpol	1179.20		NIST Webbook
tb	748.48	K	Joback Method
tc	929.50	K	Joback Method
tf	523.31	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.52	J/mol×K	748.48	Joback Method
cpg	695.46	J/mol×K	778.65	Joback Method
cpg	705.50	J/mol×K	808.82	Joback Method
cpg	714.70	J/mol×K	838.99	Joback Method
cpg	723.09	J/mol×K	869.16	Joback Method
cpg	730.71	J/mol×K	899.33	Joback Method
cpg	737.59	J/mol×K	929.50	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=U380253&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