1,5-Anhydro-D-sorbitol, tetrakis(trifluoroacetate)

Inchi: InChI=1S/C14H8F12O9/c15-11(16,17)7(27)32-1-3-5(34-9(29)13(21,22)23)6(35-10(30)14
InchiKey: MBBRCPSEFKECJI-UHFFFAOYSA-N
Formula: C14H8F12O9
SMILES: O=C(OCC1OCC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 548.19

Physical Properties

Property code	Value	Unit	Source
gf	-3279.84	kJ/mol	Joback Method
hf	-3838.51	kJ/mol	Joback Method
hfus	53.49	kJ/mol	Joback Method
hvap	72.41	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	1.913		Crippen Method
mcvol	254.130	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	1238.80		NIST Webbook
rinpol	1238.80		NIST Webbook
tb	835.69	K	Joback Method
tc	1023.43	K	Joback Method
tf	574.17	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.84	J/mol×K	835.69	Joback Method
cpg	856.74	J/mol×K	866.98	Joback Method
cpg	865.54	J/mol×K	898.27	Joback Method
cpg	873.28	J/mol×K	929.56	Joback Method
cpg	879.98	J/mol×K	960.85	Joback Method
cpg	885.69	J/mol×K	992.14	Joback Method
cpg	890.43	J/mol×K	1023.43	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=U380212&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