Sorbitol, 3-methyl, TFA

Inchi: InChI=1S/C17H11F15O11/c1-38-6(4(41-10(35)15(24,25)26)2-39-8(33)13(18,19)20)7(43-
InchiKey: BTRVHTRLEJFASW-VZFHVOOUSA-N
Formula: C17H11F15O11
SMILES: COC(C(COC(=O)C(F)(F)F)OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)OC
Mol. weight [g/mol]: 676.24

Physical Properties

Property code	Value	Unit	Source
gf	-4100.05	kJ/mol	Joback Method
hf	-4756.95	kJ/mol	Joback Method
hfus	49.95	kJ/mol	Joback Method
hvap	81.34	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	2.635		Crippen Method
mcvol	320.010	ml/mol	McGowan Method
pc	985.78	kPa	Joback Method
rinpol	1174.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1174.00		NIST Webbook
tb	963.37	K	Joback Method
tc	1202.74	K	Joback Method
tf	625.33	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1060.53	J/mol×K	963.37	Joback Method
cpg	1068.63	J/mol×K	1003.26	Joback Method
cpg	1075.19	J/mol×K	1043.16	Joback Method
cpg	1080.32	J/mol×K	1083.05	Joback Method
cpg	1084.11	J/mol×K	1122.95	Joback Method
cpg	1086.67	J/mol×K	1162.84	Joback Method
cpg	1088.10	J/mol×K	1202.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R527794&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