Sorbitol, 2,6-dimethyl, TFA

Inchi: InChI=1S/C16H14F12O10/c1-33-3-6(36-10(30)14(20,21)22)8(38-12(32)16(26,27)28)7(37
InchiKey: DIZQCSSEHCRSET-YWIQKCBGSA-N
Formula: C16H14F12O10
SMILES: COCC(OC(=O)C(F)(F)F)C(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]: 594.26

Physical Properties

Property code	Value	Unit	Source
gf	-3397.96	kJ/mol	Joback Method
hf	-4026.65	kJ/mol	Joback Method
hfus	43.93	kJ/mol	Joback Method
hvap	76.11	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.176		Crippen Method
mcvol	299.040	ml/mol	McGowan Method
pc	1084.92	kPa	Joback Method
rinpol	1237.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1226.00		NIST Webbook
tb	892.04	K	Joback Method
tc	1097.25	K	Joback Method
tf	559.94	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.41	J/mol×K	892.04	Joback Method
cpg	987.41	J/mol×K	926.24	Joback Method
cpg	996.15	J/mol×K	960.44	Joback Method
cpg	1003.66	J/mol×K	994.65	Joback Method
cpg	1010.00	J/mol×K	1028.85	Joback Method
cpg	1015.20	J/mol×K	1063.05	Joback Method
cpg	1019.30	J/mol×K	1097.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R527709&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