D-(-)-Tagatofuranose, pentakis(trifluoroacetate) (isomer 2)

Inchi: InChI=1S/C16H7F15O11/c17-12(18,19)6(32)37-1-3-4(39-8(34)14(23,24)25)5(40-9(35)15
InchiKey: XZVKUTGQYBCICM-UHFFFAOYSA-N
Formula: C16H7F15O11
SMILES: O=C(OCC1OC(COC(=O)C(F)(F)F)(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(
Mol. weight [g/mol]: 660.20

Physical Properties

Property code	Value	Unit	Source
gf	-4071.90	kJ/mol	Joback Method
hf	-4700.27	kJ/mol	Joback Method
hfus	59.09	kJ/mol	Joback Method
hvap	80.94	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.346		Crippen Method
mcvol	295.060	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	1308.80		NIST Webbook
tb	948.29	K	Joback Method
tc	1170.12	K	Joback Method
tf	700.48	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.35	J/mol×K	948.29	Joback Method
cpg	1021.57	J/mol×K	985.26	Joback Method
cpg	1032.33	J/mol×K	1022.23	Joback Method
cpg	1042.81	J/mol×K	1059.20	Joback Method
cpg	1053.18	J/mol×K	1096.18	Joback Method
cpg	1063.59	J/mol×K	1133.15	Joback Method
cpg	1074.22	J/mol×K	1170.12	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=U380299&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