D-(+)-Talofuranose, pentakis(trifluoroacetate) (isomer 1)

Inchi: InChI=1S/C16H7F15O11/c17-12(18,19)7(32)37-1-2(38-8(33)13(20,21)22)3-4(40-9(34)14
InchiKey: NPUHIXXXZHPNAB-UHFFFAOYSA-N
Formula: C16H7F15O11
SMILES: O=C(OCC(OC(=O)C(F)(F)F)C1OC(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	-4068.85	kJ/mol	Joback Method
hf	-4720.79	kJ/mol	Joback Method
hfus	61.86	kJ/mol	Joback Method
hvap	81.71	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	2.345		Crippen Method
mcvol	295.060	ml/mol	McGowan Method
pc	1093.54	kPa	Joback Method
rinpol	1188.10		NIST Webbook
tb	947.61	K	Joback Method
tc	1170.59	K	Joback Method
tf	661.58	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1008.82	J/mol×K	947.61	Joback Method
cpg	1016.42	J/mol×K	984.77	Joback Method
cpg	1022.58	J/mol×K	1021.94	Joback Method
cpg	1027.40	J/mol×K	1059.10	Joback Method
cpg	1030.94	J/mol×K	1096.27	Joback Method
cpg	1033.28	J/mol×K	1133.43	Joback Method
cpg	1034.50	J/mol×K	1170.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380270&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