D-Fructopyranose, pentakis(trifluoroacetate)

Other names: D-(-)-Fructopyranose, pentakis(trifluoroacetate) (isomer 2)
Inchi: InChI=1S/C16H7F15O11/c17-12(18,19)6(32)37-2-11(42-10(36)16(29,30)31)5(41-9(35)15
InchiKey: TVXVQZUZYLRUBY-UHFFFAOYSA-N
Formula: C16H7F15O11
SMILES: O=C(OCC1(OC(=O)C(F)(F)F)OCC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(
Mol. weight [g/mol]: 660.20
CAS: 56942-38-2

Physical Properties

Property code	Value	Unit	Source
gf	-4084.00	kJ/mol	Joback Method
hf	-4706.43	kJ/mol	Joback Method
hfus	56.99	kJ/mol	Joback Method
hvap	81.12	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.346		Crippen Method
mcvol	295.060	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	1161.70		NIST Webbook
rinpol	1161.70		NIST Webbook
tb	952.56	K	Joback Method
tc	1173.44	K	Joback Method
tf	696.96	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.67	J/mol×K	952.56	Joback Method
cpg	1024.63	J/mol×K	989.37	Joback Method
cpg	1035.04	J/mol×K	1026.19	Joback Method
cpg	1045.07	J/mol×K	1063.00	Joback Method
cpg	1054.87	J/mol×K	1099.82	Joback Method
cpg	1064.59	J/mol×K	1136.63	Joback Method

cpg	1074.39	J/mol×K	1173.44	Joback Method

Sources

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=C56942382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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