D-(+)-Glucose, pentakis(trifluoroacetate) (isomer 2)

Inchi: InChI=1S/C16H7F15O11/c17-12(18,19)7(32)37-1-2-3(39-8(33)13(20,21)22)4(40-9(34)14
InchiKey: FMTKBUZWITYHQE-UHFFFAOYSA-N
Formula: C16H7F15O11
SMILES: O=C(OCC1OC(OC(=O)C(F)(F)F)C(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	-4086.22	kJ/mol	Joback Method
hf	-4742.01	kJ/mol	Joback Method
hfus	64.36	kJ/mol	Joback Method
hvap	81.96	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	2.345		Crippen Method
mcvol	295.060	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	1177.60		NIST Webbook
rinpol	1177.60		NIST Webbook
tb	947.65	K	Joback Method
tc	1169.63	K	Joback Method
tf	668.82	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1016.80	J/mol×K	947.65	Joback Method
cpg	1024.35	J/mol×K	984.65	Joback Method
cpg	1030.30	J/mol×K	1021.64	Joback Method
cpg	1034.72	J/mol×K	1058.64	Joback Method
cpg	1037.66	J/mol×K	1095.64	Joback Method
cpg	1039.18	J/mol×K	1132.63	Joback Method
cpg	1039.34	J/mol×K	1169.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380257&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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