Benzyl «beta»-D-glucopyranoside, TFA

Inchi: InChI=1S/C22H16F12O9/c23-19(24,25)11(35)7-6-10-12(41-16(36)20(26,27)28)13(42-17
InchiKey: YLORDZKJSTYSMF-DJIJKHNZSA-N
Formula: C22H16F12O9
SMILES: O=C(CCC1OC(OCc2ccccc2)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 652.34

Physical Properties

Property code	Value	Unit	Source
gf	-3107.78	kJ/mol	Joback Method
hf	-3787.44	kJ/mol	Joback Method
hfus	69.33	kJ/mol	Joback Method
hvap	92.18	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	4.262		Crippen Method
mcvol	343.090	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
rinpol	1751.00		NIST Webbook
rinpol	1746.00		NIST Webbook
tb	1040.74	K	Joback Method
tc	1284.09	K	Joback Method
tf	686.51	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1197.78	J/mol×K	1040.74	Joback Method
cpg	1205.73	J/mol×K	1081.30	Joback Method
cpg	1211.84	J/mol×K	1121.86	Joback Method
cpg	1216.21	J/mol×K	1162.42	Joback Method
cpg	1218.96	J/mol×K	1202.98	Joback Method
cpg	1220.17	J/mol×K	1243.53	Joback Method
cpg	1219.97	J/mol×K	1284.09	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=R330451&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