Benzoyl glucopyranoside, isomer # 3, TFA

Inchi: InChI=1S/C21H12F12O11/c22-18(23,24)14(35)39-6-8-9(41-15(36)19(25,26)27)10(42-16
InchiKey: OIHUEIHTIVWSTA-TWEVDUBQSA-N
Formula: C21H12F12O11
SMILES: O=C(OC1OC(COC(=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]: 668.29

Physical Properties

Property code	Value	Unit	Source
gf	-3350.12	kJ/mol	Joback Method
hf	-4011.60	kJ/mol	Joback Method
hfus	69.52	kJ/mol	Joback Method
hvap	99.11	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	3.096		Crippen Method
mcvol	336.440	ml/mol	McGowan Method
pc	1058.95	kPa	Joback Method
rinpol	1727.00		NIST Webbook
tb	1094.15	K	Joback Method
tc	1354.99	K	Joback Method
tf	747.40	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1159.08	J/mol×K	1094.15	Joback Method
cpg	1162.43	J/mol×K	1137.62	Joback Method
cpg	1163.55	J/mol×K	1181.10	Joback Method
cpg	1162.53	J/mol×K	1224.57	Joback Method
cpg	1159.46	J/mol×K	1268.05	Joback Method
cpg	1154.45	J/mol×K	1311.52	Joback Method
cpg	1147.58	J/mol×K	1354.99	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=R330446&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