2-Phenylethyl «beta»-D-glucopyranoside, TFA

Inchi: InChI=1S/C23H18F12O9/c24-20(25,26)12(36)7-6-11-13(42-17(37)21(27,28)29)14(43-18
InchiKey: HQUAEVKXTOFIFZ-SLZITWOASA-N
Formula: C23H18F12O9
SMILES: O=C(CCC1OC(OCCc2ccccc2)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)
Mol. weight [g/mol]: 666.36

Physical Properties

Property code	Value	Unit	Source
gf	-3099.36	kJ/mol	Joback Method
hf	-3808.08	kJ/mol	Joback Method
hfus	71.92	kJ/mol	Joback Method
hvap	94.41	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	4.304		Crippen Method
mcvol	357.180	ml/mol	McGowan Method
pc	912.18	kPa	Joback Method
rinpol	1829.00		NIST Webbook
tb	1063.62	K	Joback Method
tc	1317.79	K	Joback Method
tf	697.78	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1255.41	J/mol×K	1063.62	Joback Method
cpg	1263.38	J/mol×K	1105.98	Joback Method
cpg	1269.35	J/mol×K	1148.34	Joback Method
cpg	1273.46	J/mol×K	1190.71	Joback Method
cpg	1275.83	J/mol×K	1233.07	Joback Method
cpg	1276.58	J/mol×K	1275.43	Joback Method
cpg	1275.85	J/mol×K	1317.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R330397&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