2-Phenylethnol, «beta»-D-glucoside, TFA

Other names: Phenethyl alcohol, Gly, TFA
Phenethyl alcohol, «beta»-D-glucopyranoside, TFA
«beta»-phenylethyl «beta»-D-glucopyranoside, TFA
2-Phenyl ethanol «beta»-D-glucopyranoside, TFA

Inchi: InChI=1S/C22H16F12O10/c23-19(24,25)15(35)40-8-10-11(42-16(36)20(26,27)28)12(43-

InchiKey: NOABXVMGFIRNNW-HPCHECBXSA-N

Formula: C22H16F12O10

SMILES: O=C(OCC1OC(OCCc2ccccc2)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)

Mol. weight [g/mol]: 668.34

Physical Properties

Property code	Value	Unit	Source
gf	-3212.78	kJ/mol	Joback Method
hf	-3919.66	kJ/mol	Joback Method
hfus	70.52	kJ/mol	Joback Method
hvap	94.59	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	3.498		Crippen Method
mcvol	348.960	ml/mol	McGowan Method
pc	957.32	kPa	Joback Method
rinpol	1856.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1856.00		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	1856.00		NIST Webbook
rinpol	1856.00		NIST Webbook
rinpol	1840.00		NIST Webbook
tb	1063.16	K	Joback Method
tc	1316.55	K	Joback Method
tf	708.74	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.33	J/mol×K	1063.16	Joback Method
cpg	1226.83	J/mol×K	1105.39	Joback Method
cpg	1231.14	J/mol×K	1147.62	Joback Method
cpg	1233.38	J/mol×K	1189.86	Joback Method
cpg	1233.62	J/mol×K	1232.09	Joback Method
cpg	1231.96	J/mol×K	1274.32	Joback Method
cpg	1228.50	J/mol×K	1316.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R184857&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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