4-Phenylbutan-2-ol trifluoroacetate

Other names:	2-Butanol, 4-phenyl-O-trifluoroacetyl-
	2-trifluoroacetyloxy-4-phenylbutane
	4-Phenyl-2-butanol trifluoroacetate
Inchi:	InChI=1S/C12H13F3O2/c1-9(17-11(16)12(13,14)15)7-8-10-5-3-2-4-6-10/h2-6,9H,7-8H2,1
InchiKey:	RCNPYDZVSNUILB-UHFFFAOYSA-N
Formula:	C12H13F3O2
SMILES:	CC(CCc1ccccc1)OC(=O)C(F)(F)F
Mol. weight [g/mol]:	246.23

Physical Properties

Property code
af
gf
hf
hfus
hvap
ie
log10ws
logp
mcvol

pc
rinpol
tb
tc
tf
vc

Temperature Dependent Properties

Property code
cpg
cpg
cpg
cpg
cpg
cpg
cpg

Sources

Cheméo Relay (1.0):	https://www.chemeo.com
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U372995&Units=SI
Cheméo Relay (1.0, beta):	https://www.chemeo.com

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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