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,
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	Value	Unit	Source
gf	-655.38	kJ/mol	Joback Method
hf	-901.64	kJ/mol	Joback Method
hfus	21.97	kJ/mol	Joback Method
hvap	49.60	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.113		Crippen Method
mcvol	168.930	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1229.00		NIST Webbook
tb	571.07	K	Joback Method
tc	764.43	K	Joback Method
tf	312.77	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.21	J/mol×K	571.07	Joback Method
cpg	436.46	J/mol×K	603.30	Joback Method
cpg	449.83	J/mol×K	635.52	Joback Method
cpg	462.35	J/mol×K	667.75	Joback Method
cpg	474.05	J/mol×K	699.97	Joback Method
cpg	484.98	J/mol×K	732.20	Joback Method

cpg	495.17	J/mol×K	764.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U372995&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

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