4-Hydroxyphenethyl alcohol, bis(trifluoroacetate)

Inchi: InChI=1S/C12H8F6O4/c13-11(14,15)9(19)21-6-5-7-1-3-8(4-2-7)22-10(20)12(16,17)18/h1

InchiKey: POXBHGCPRHUJSJ-UHFFFAOYSA-N

Formula: C12H8F6O4

SMILES: O=C(OCCc1ccc(OC(=O)C(F)(F)F)cc1)C(F)(F)F

Mol. weight [g/mol]: 330.18

Physical Properties

Property code	Value	Unit	Source
gf	-1478.08	kJ/mol	Joback Method
hf	-1749.71	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	56.06	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	2.802		Crippen Method
mcvol	181.680	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	1288.00		NIST Webbook
tb	647.36	K	Joback Method
tc	830.71	K	Joback Method
tf	416.64	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.43	J/mol×K	647.36	Joback Method
cpg	502.34	J/mol×K	677.92	Joback Method
cpg	512.49	J/mol×K	708.48	Joback Method
cpg	521.91	J/mol×K	739.03	Joback Method
cpg	530.64	J/mol×K	769.59	Joback Method
cpg	538.71	J/mol×K	800.15	Joback Method
cpg	546.14	J/mol×K	830.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376199&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

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