4-Hydroxyphenethyl alcohol, bis(pentafluoropropionate)

Inchi: InChI=1S/C14H8F10O4/c15-11(16,13(19,20)21)9(25)27-6-5-7-1-3-8(4-2-7)28-10(26)12(1

InchiKey: VBEIAWKZVNXVMQ-UHFFFAOYSA-N

Formula: C14H8F10O4

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

Mol. weight [g/mol]: 430.19

Physical Properties

Property code	Value	Unit	Source
gf	-2234.80	kJ/mol	Joback Method
hf	-2592.93	kJ/mol	Joback Method
hfus	32.39	kJ/mol	Joback Method
hvap	54.65	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.073		Crippen Method
mcvol	216.940	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinpol	1317.00		NIST Webbook
rinpol	1317.00		NIST Webbook
tb	683.74	K	Joback Method
tc	856.45	K	Joback Method
tf	446.38	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.71	J/mol×K	683.74	Joback Method
cpg	641.41	J/mol×K	712.53	Joback Method
cpg	651.28	J/mol×K	741.31	Joback Method
cpg	660.38	J/mol×K	770.10	Joback Method
cpg	668.76	J/mol×K	798.88	Joback Method
cpg	676.47	J/mol×K	827.67	Joback Method
cpg	683.57	J/mol×K	856.45	Joback Method

Sources

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=U376198&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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