2-(2-Hydroxyethoxy)phenol, bis(pentafluoropropionate)

Inchi: InChI=1S/C14H8F10O5/c15-11(16,13(19,20)21)9(25)28-6-5-27-7-3-1-2-4-8(7)29-10(26)1

InchiKey: PUXFXNXGJJOULV-UHFFFAOYSA-N

Formula: C14H8F10O5

SMILES: O=C(OCCOc1ccccc1OC(=O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 446.19

Physical Properties

Property code	Value	Unit	Source
gf	-2339.80	kJ/mol	Joback Method
hf	-2725.15	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	57.06	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	3.909		Crippen Method
mcvol	222.810	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	1375.00		NIST Webbook
tb	706.16	K	Joback Method
tc	879.82	K	Joback Method
tf	468.61	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.04	J/mol×K	706.16	Joback Method
cpg	666.47	J/mol×K	735.10	Joback Method
cpg	676.10	J/mol×K	764.05	Joback Method
cpg	684.95	J/mol×K	792.99	Joback Method
cpg	693.10	J/mol×K	821.93	Joback Method
cpg	700.57	J/mol×K	850.87	Joback Method
cpg	707.41	J/mol×K	879.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376169&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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