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

Inchi: InChI=1S/C16H8F14O5/c17-11(18,13(21,22)15(25,26)27)9(31)34-6-5-33-7-3-1-2-4-8(7)3

InchiKey: RNBODFJLGRZVJQ-UHFFFAOYSA-N

Formula: C16H8F14O5

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

Mol. weight [g/mol]: 546.21

Physical Properties

Property code	Value	Unit	Source
gf	-3096.52	kJ/mol	Joback Method
hf	-3568.37	kJ/mol	Joback Method
hfus	36.25	kJ/mol	Joback Method
hvap	55.66	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.180		Crippen Method
mcvol	258.070	ml/mol	McGowan Method
pc	1206.47	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
tb	742.54	K	Joback Method
tc	913.28	K	Joback Method
tf	498.35	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.76	J/mol×K	742.54	Joback Method
cpg	807.92	J/mol×K	771.00	Joback Method
cpg	817.22	J/mol×K	799.45	Joback Method
cpg	825.74	J/mol×K	827.91	Joback Method
cpg	833.55	J/mol×K	856.37	Joback Method
cpg	840.71	J/mol×K	884.82	Joback Method
cpg	847.29	J/mol×K	913.28	Joback Method

Sources

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=U376168&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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