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

Inchi: InChI=1S/C12H8F6O5/c13-11(14,15)9(19)22-6-5-21-7-3-1-2-4-8(7)23-10(20)12(16,17)18

InchiKey: TVWIAUGNKIYKJD-UHFFFAOYSA-N

Formula: C12H8F6O5

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

Mol. weight [g/mol]: 346.18

Physical Properties

Property code	Value	Unit	Source
gf	-1583.08	kJ/mol	Joback Method
hf	-1881.93	kJ/mol	Joback Method
hfus	30.90	kJ/mol	Joback Method
hvap	58.47	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.639		Crippen Method
mcvol	187.550	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	1355.00		NIST Webbook
rinpol	1355.00		NIST Webbook
tb	669.78	K	Joback Method
tc	852.67	K	Joback Method
tf	438.87	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.01	J/mol×K	669.78	Joback Method
cpg	526.69	J/mol×K	700.26	Joback Method
cpg	536.63	J/mol×K	730.74	Joback Method
cpg	545.86	J/mol×K	761.22	Joback Method
cpg	554.39	J/mol×K	791.70	Joback Method
cpg	562.24	J/mol×K	822.19	Joback Method
cpg	569.44	J/mol×K	852.67	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=U376170&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