2-Propanol, 1,1,1,3,3,3-hexafluoro-2-[2-(1-methylethyl)phenoxy

Inchi: InChI=1S/C12H12F6O2/c1-7(2)8-5-3-4-6-9(8)20-10(19,11(13,14)15)12(16,17)18/h3-7,19

InchiKey: DGWCUQRDBNRYAK-UHFFFAOYSA-N

Formula: C12H12F6O2

SMILES: CC(C)c1ccccc1OC(O)(C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 302.21

CAS: 52447-66-2

Physical Properties

Property code	Value	Unit	Source
gf	-1251.66	kJ/mol	Joback Method
hf	-1558.59	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	55.16	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.002		Crippen Method
mcvol	178.540	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
tb	605.71	K	Joback Method
tc	779.30	K	Joback Method
tf	342.79	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.23	J/mol×K	605.71	Joback Method
cpg	503.30	J/mol×K	634.64	Joback Method
cpg	514.54	J/mol×K	663.57	Joback Method
cpg	525.02	J/mol×K	692.51	Joback Method
cpg	534.77	J/mol×K	721.44	Joback Method
cpg	543.85	J/mol×K	750.37	Joback Method
cpg	552.30	J/mol×K	779.30	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=C52447662&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume