4,4'-BIS[2-HYDROXYHEXAFLUOROISOPROPYL]DIPHENYL ETHER

InChI: InChI=1S/C18H10F12O3/c19-15(20,21)13(31,16(22,23)24)9-1-5-11(6-2-9)33-12-7-3-10(4

InchiKey: PRBPSTYDUVSNOK-UHFFFAOYSA-N

Formula: C18H10F12O3

SMILES: OC(c1ccc(Oc2ccc(C(O)(C(F)(F)F)C(F)(F)F)cc2)cc1)(C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 502.25

Physical Properties

Property code	Value	Unit	Source
hfus	31.52	kJ/mol	Joback Method
logp	6.103		Crippen Method
mcvol	255.810	ml/mol	McGowan Method
tb	596.52	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.85	J/mol×K	853.20	Joback Method
cpg	827.43	J/mol×K	885.19	Joback Method
cpg	835.43	J/mol×K	917.18	Joback Method
cpg	842.97	J/mol×K	949.17	Joback Method
cpg	850.18	J/mol×K	981.16	Joback Method
cpg	857.20	J/mol×K	1013.15	Joback Method
cpg	864.15	J/mol×K	1045.14	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2093041&Units=SI

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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature