4,4'-Bis(2-hydroxyhexafluoroisopropyl)diphenyl

Inchi: InChI=1S/C18H10F12O2/c19-15(20,21)13(31,16(22,23)24)11-5-1-9(2-6-11)10-3-7-12(8-
InchiKey: JCNFGVSJUHFARO-UHFFFAOYSA-N
Formula: C18H10F12O2
SMILES: OC(c1ccc(-c2ccc(C(O)(C(F)(F)F)C(F)(F)F)cc2)cc1)(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 486.25
CAS: 2180-30-5

Physical Properties

Property code	Value	Unit	Source
gf	-2288.08	kJ/mol	Joback Method
hf	-2675.01	kJ/mol	Joback Method
hfus	30.33	kJ/mol	Joback Method
hvap	77.32	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	5.978		Crippen Method
mcvol	249.940	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
tb	830.78	K	Joback Method
tc	1018.92	K	Joback Method
tf	513.74	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.22	J/mol×K	830.78	Joback Method
cpg	802.91	J/mol×K	862.14	Joback Method
cpg	811.01	J/mol×K	893.49	Joback Method
cpg	818.63	J/mol×K	924.85	Joback Method
cpg	825.93	J/mol×K	956.21	Joback Method
cpg	833.04	J/mol×K	987.56	Joback Method
cpg	840.08	J/mol×K	1018.92	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=C2180305&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume