Fumaric acid, 2-isopropoxyphenyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C18H16F8O5/c1-10(2)30-11-5-3-4-6-12(11)31-14(28)8-7-13(27)29-9-16(21,22
InchiKey: FGZCOVXFCXJZBE-BQYQJAHWSA-N
Formula: C18H16F8O5
SMILES: CC(C)Oc1ccccc1OC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 464.30

Physical Properties

Property code	Value	Unit	Source
gf	-1844.00	kJ/mol	Joback Method
hf	-2300.08	kJ/mol	Joback Method
hfus	38.34	kJ/mol	Joback Method
hvap	68.08	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.650		Crippen Method
mcvol	271.330	ml/mol	McGowan Method
pc	1284.67	kPa	Joback Method
rinpol	1967.00		NIST Webbook
rinpol	1967.00		NIST Webbook
tb	805.65	K	Joback Method
tc	994.15	K	Joback Method
tf	475.01	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.86	J/mol×K	805.65	Joback Method
cpg	841.95	J/mol×K	837.07	Joback Method
cpg	853.14	J/mol×K	868.48	Joback Method
cpg	863.46	J/mol×K	899.90	Joback Method
cpg	873.00	J/mol×K	931.32	Joback Method
cpg	881.81	J/mol×K	962.73	Joback Method
cpg	889.95	J/mol×K	994.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U405708&Units=SI

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