Succinic acid, 2-isopropoxyphenyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C17H17F7O5/c1-10(2)28-11-5-3-4-6-12(11)29-14(26)8-7-13(25)27-9-15(18,19

InchiKey: QUWWLORUNZEJPD-UHFFFAOYSA-N

Formula: C17H17F7O5

SMILES: CC(C)Oc1ccccc1OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 434.30

Physical Properties

Property code	Value	Unit	Source
gf	-1735.39	kJ/mol	Joback Method
hf	-2195.27	kJ/mol	Joback Method
hfus	35.99	kJ/mol	Joback Method
hvap	67.10	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.535		Crippen Method
mcvol	259.770	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	1844.00		NIST Webbook
tb	779.78	K	Joback Method
tc	965.47	K	Joback Method
tf	483.23	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.80	J/mol×K	779.78	Joback Method
cpg	804.38	J/mol×K	810.73	Joback Method
cpg	816.03	J/mol×K	841.68	Joback Method
cpg	826.80	J/mol×K	872.63	Joback Method
cpg	836.72	J/mol×K	903.57	Joback Method
cpg	845.86	J/mol×K	934.52	Joback Method
cpg	854.25	J/mol×K	965.47	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=U357965&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume