Succinic acid, 2-isopropoxyphenyl pentafluorobenzyl ester

Inchi: InChI=1S/C20H17F5O5/c1-10(2)29-12-5-3-4-6-13(12)30-15(27)8-7-14(26)28-9-11-16(21

InchiKey: WCTHNQBXUOLTIR-UHFFFAOYSA-N

Formula: C20H17F5O5

SMILES: CC(C)Oc1ccccc1OC(=O)CCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 432.34

Physical Properties

Property code	Value	Unit	Source
gf	-1264.77	kJ/mol	Joback Method
hf	-1659.54	kJ/mol	Joback Method
hfus	51.94	kJ/mol	Joback Method
hvap	84.89	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	4.598		Crippen Method
mcvol	274.740	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	2409.00		NIST Webbook
rinpol	2409.00		NIST Webbook
tb	911.15	K	Joback Method
tc	1119.22	K	Joback Method
tf	597.62	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.97	J/mol×K	911.15	Joback Method
cpg	850.21	J/mol×K	945.83	Joback Method
cpg	860.21	J/mol×K	980.51	Joback Method
cpg	868.96	J/mol×K	1015.19	Joback Method
cpg	876.47	J/mol×K	1049.87	Joback Method
cpg	882.72	J/mol×K	1084.54	Joback Method
cpg	887.70	J/mol×K	1119.22	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=U357972&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume