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

Inchi: InChI=1S/C17H17F7O4/c1-10(2)11-3-5-12(6-4-11)28-14(26)8-7-13(25)27-9-15(18,19)16

InchiKey: CSYKNNSZXLQVBV-UHFFFAOYSA-N

Formula: C17H17F7O4

SMILES: CC(C)c1ccc(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F)cc1

Mol. weight [g/mol]: 418.30

Physical Properties

Property code	Value	Unit	Source
gf	-1630.39	kJ/mol	Joback Method
hf	-2063.05	kJ/mol	Joback Method
hfus	34.81	kJ/mol	Joback Method
hvap	64.69	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.872		Crippen Method
mcvol	253.900	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	1843.00		NIST Webbook
tb	757.36	K	Joback Method
tc	941.79	K	Joback Method
tf	461.00	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.57	J/mol×K	757.36	Joback Method
cpg	777.46	J/mol×K	788.10	Joback Method
cpg	789.43	J/mol×K	818.84	Joback Method
cpg	800.54	J/mol×K	849.57	Joback Method
cpg	810.84	J/mol×K	880.31	Joback Method
cpg	820.39	J/mol×K	911.05	Joback Method
cpg	829.24	J/mol×K	941.79	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=U360713&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