Succinic acid, di(2,3,4,5-tetrafluorobenzyl) ester

Inchi: InChI=1S/C18H10F8O4/c19-9-3-7(13(21)17(25)15(9)23)5-29-11(27)1-2-12(28)30-6-8-4-10(20)14(22)18(26)16(8)24

InchiKey: HACVIYPOQDTULW-UHFFFAOYSA-N

Formula: C18H10F8O4

SMILES: O=C(CCC(=O)OCc1cc(F)c(F)c(F)c1F)OCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 442.26

Physical Properties

Property code	Value	Unit	Source
gf	-1777.86	kJ/mol	Joback Method
hf	-2092.03	kJ/mol	Joback Method
hfus	57.56	kJ/mol	Joback Method
hvap	77.29	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	4.366		Crippen Method
mcvol	246.000	ml/mol	McGowan Method
pc	1400.64	kPa	Joback Method
rinpol	2181.00		NIST Webbook
rinpol	2181.00		NIST Webbook
tb	851.18	K	Joback Method
tc	1045.17	K	Joback Method
tf	594.66	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.65	J/mol×K	851.18	Joback Method
cpg	728.86	J/mol×K	883.51	Joback Method
cpg	738.18	J/mol×K	915.84	Joback Method
cpg	746.60	J/mol×K	948.17	Joback Method
cpg	754.11	J/mol×K	980.51	Joback Method
cpg	760.70	J/mol×K	1012.84	Joback Method
cpg	766.39	J/mol×K	1045.17	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=U381627&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