Succinic acid, 2-methylhex-3-yl 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C18H22F4O4/c1-4-5-13(10(2)3)26-15(24)7-6-14(23)25-9-11-8-12(19)17(21)18

InchiKey: ISQGZYVRRPXLDH-UHFFFAOYSA-N

Formula: C18H22F4O4

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

Mol. weight [g/mol]: 378.36

Physical Properties

Property code	Value	Unit	Source
gf	-1077.39	kJ/mol	Joback Method
hf	-1508.80	kJ/mol	Joback Method
hfus	45.71	kJ/mol	Joback Method
hvap	74.85	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.434		Crippen Method
mcvol	262.680	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook
tb	806.62	K	Joback Method
tc	995.17	K	Joback Method
tf	485.80	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.17	J/mol×K	806.62	Joback Method
cpg	804.19	J/mol×K	838.05	Joback Method
cpg	817.27	J/mol×K	869.47	Joback Method
cpg	829.42	J/mol×K	900.90	Joback Method
cpg	840.64	J/mol×K	932.32	Joback Method
cpg	850.94	J/mol×K	963.75	Joback Method
cpg	860.32	J/mol×K	995.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381615&Units=SI
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

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

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