Succinic acid, pentyl 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C16H18F4O4/c1-2-3-4-7-23-12(21)5-6-13(22)24-9-10-8-11(17)15(19)16(20)14

InchiKey: XYCGXDDLLDBWPJ-UHFFFAOYSA-N

Formula: C16H18F4O4

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

Mol. weight [g/mol]: 350.31

Physical Properties

Property code	Value	Unit	Source
gf	-1089.35	kJ/mol	Joback Method
hf	-1456.96	kJ/mol	Joback Method
hfus	47.57	kJ/mol	Joback Method
hvap	71.18	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	3.800		Crippen Method
mcvol	234.500	ml/mol	McGowan Method
pc	1512.85	kPa	Joback Method
rinpol	1946.00		NIST Webbook
rinpol	1946.00		NIST Webbook
tb	761.74	K	Joback Method
tc	944.71	K	Joback Method
tf	493.26	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.72	J/mol×K	761.74	Joback Method
cpg	689.69	J/mol×K	792.24	Joback Method
cpg	701.88	J/mol×K	822.73	Joback Method
cpg	713.30	J/mol×K	853.23	Joback Method
cpg	723.94	J/mol×K	883.72	Joback Method
cpg	733.81	J/mol×K	914.22	Joback Method
cpg	742.90	J/mol×K	944.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381614&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