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

Inchi: InChI=1S/C23H32F4O4/c1-2-3-4-5-6-7-8-9-10-11-14-30-19(28)12-13-20(29)31-16-17-15

InchiKey: JZXKIITXLNNYKD-UHFFFAOYSA-N

Formula: C23H32F4O4

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

Mol. weight [g/mol]: 448.49

Physical Properties

Property code	Value	Unit	Source
gf	-1030.41	kJ/mol	Joback Method
hf	-1601.44	kJ/mol	Joback Method
hfus	65.70	kJ/mol	Joback Method
hvap	86.76	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	6.530		Crippen Method
mcvol	333.130	ml/mol	McGowan Method
pc	950.84	kPa	Joback Method
rinpol	2637.00		NIST Webbook
rinpol	2637.00		NIST Webbook
tb	921.90	K	Joback Method
tc	1129.90	K	Joback Method
tf	572.15	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.50	J/mol×K	921.90	Joback Method
cpg	1100.45	J/mol×K	956.57	Joback Method
cpg	1115.07	J/mol×K	991.23	Joback Method
cpg	1128.36	J/mol×K	1025.90	Joback Method
cpg	1140.36	J/mol×K	1060.57	Joback Method
cpg	1151.07	J/mol×K	1095.23	Joback Method
cpg	1160.53	J/mol×K	1129.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381622&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