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

Inchi: InChI=1S/C25H36F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-32-21(30)14-15-22(31)33-18

InchiKey: KSJIHBGAPWSSPY-UHFFFAOYSA-N

Formula: C25H36F4O4

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

Mol. weight [g/mol]: 476.54

Physical Properties

Property code	Value	Unit	Source
gf	-1013.57	kJ/mol	Joback Method
hf	-1642.72	kJ/mol	Joback Method
hfus	70.89	kJ/mol	Joback Method
hvap	91.21	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	7.311		Crippen Method
mcvol	361.310	ml/mol	McGowan Method
pc	847.51	kPa	Joback Method
rinpol	2838.00		NIST Webbook
rinpol	2838.00		NIST Webbook
tb	967.66	K	Joback Method
tc	1191.37	K	Joback Method
tf	594.69	K	Joback Method
vc	1.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1207.00	J/mol×K	967.66	Joback Method
cpg	1223.88	J/mol×K	1004.95	Joback Method
cpg	1239.14	J/mol×K	1042.23	Joback Method
cpg	1252.81	J/mol×K	1079.52	Joback Method
cpg	1264.93	J/mol×K	1116.80	Joback Method
cpg	1275.52	J/mol×K	1154.09	Joback Method
cpg	1284.63	J/mol×K	1191.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381624&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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