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

Inchi: InChI=1S/C26H38F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-33-22(31)15-16-23(32)34
InchiKey: QNKPKEUFSDBLGI-UHFFFAOYSA-N
Formula: C26H38F4O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]: 490.57

Physical Properties

Property code	Value	Unit	Source
gf	-1005.15	kJ/mol	Joback Method
hf	-1663.36	kJ/mol	Joback Method
hfus	73.48	kJ/mol	Joback Method
hvap	93.44	kJ/mol	Joback Method
log10ws	-9.36		Crippen Method
logp	7.701		Crippen Method
mcvol	375.400	ml/mol	McGowan Method
pc	802.06	kPa	Joback Method
rinpol	2938.00		NIST Webbook
rinpol	2938.00		NIST Webbook
tb	990.54	K	Joback Method
tc	1223.94	K	Joback Method
tf	605.96	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1268.94	J/mol×K	990.54	Joback Method
cpg	1286.31	J/mol×K	1029.44	Joback Method
cpg	1301.88	J/mol×K	1068.34	Joback Method
cpg	1315.70	J/mol×K	1107.24	Joback Method
cpg	1327.82	J/mol×K	1146.14	Joback Method
cpg	1338.26	J/mol×K	1185.04	Joback Method
cpg	1347.08	J/mol×K	1223.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381625&Units=SI

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