Succinic acid, pentadecyl 3,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C26H39F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-32-24(30)15-16-25(31)33
InchiKey: KFSIBSMNLUVKJU-UHFFFAOYSA-N
Formula: C26H39F3O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCc1cc(F)c(F)c(F)c1
Mol. weight [g/mol]: 472.58

Physical Properties

Property code	Value	Unit	Source
gf	-800.71	kJ/mol	Joback Method
hf	-1455.78	kJ/mol	Joback Method
hfus	70.78	kJ/mol	Joback Method
hvap	93.59	kJ/mol	Joback Method
log10ws	-9.02		Crippen Method
logp	7.562		Crippen Method
mcvol	373.630	ml/mol	McGowan Method
pc	830.02	kPa	Joback Method
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook
tb	986.29	K	Joback Method
tc	1214.66	K	Joback Method
tf	592.85	K	Joback Method
vc	1.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1262.84	J/mol×K	986.29	Joback Method
cpg	1280.22	J/mol×K	1024.35	Joback Method
cpg	1295.89	J/mol×K	1062.41	Joback Method
cpg	1309.92	J/mol×K	1100.47	Joback Method
cpg	1322.34	J/mol×K	1138.54	Joback Method
cpg	1333.20	J/mol×K	1176.60	Joback Method
cpg	1342.54	J/mol×K	1214.66	Joback Method

Sources

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=U382199&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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