Succinic acid, tridecyl 4-trifluoromethylbenzyl ester

Inchi: InChI=1S/C25H37F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-19-31-23(29)17-18-24(30)32-20-21
InchiKey: GVZCCAJDKKBQNV-UHFFFAOYSA-N
Formula: C25H37F3O4
SMILES: CCCCCCCCCCCCCOC(=O)CCC(=O)OCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 458.55

Physical Properties

Property code	Value	Unit	Source
gf	-787.03	kJ/mol	Joback Method
hf	-1420.95	kJ/mol	Joback Method
hfus	61.56	kJ/mol	Joback Method
hvap	88.75	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.383		Crippen Method
mcvol	359.540	ml/mol	McGowan Method
pc	903.97	kPa	Joback Method
rinpol	2801.00		NIST Webbook
rinpol	2801.00		NIST Webbook
tb	950.22	K	Joback Method
tc	1164.31	K	Joback Method
tf	558.96	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1202.08	J/mol×K	950.22	Joback Method
cpg	1218.96	J/mol×K	985.90	Joback Method
cpg	1234.49	J/mol×K	1021.58	Joback Method
cpg	1248.74	J/mol×K	1057.26	Joback Method
cpg	1261.79	J/mol×K	1092.94	Joback Method
cpg	1273.68	J/mol×K	1128.63	Joback Method
cpg	1284.51	J/mol×K	1164.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382450&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