Succinic acid, 2-fluoro-6-(trifluoromethyl)benzyl tridecyl ester

Inchi: InChI=1S/C25H36F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-18-32-23(30)16-17-24(31)33-19-20
InchiKey: MEHPUNDGUVASEY-UHFFFAOYSA-N
Formula: C25H36F4O4
SMILES: CCCCCCCCCCCCCOC(=O)CCC(=O)OCc1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 476.54

Physical Properties

Property code	Value	Unit	Source
gf	-991.47	kJ/mol	Joback Method
hf	-1628.53	kJ/mol	Joback Method
hfus	64.25	kJ/mol	Joback Method
hvap	88.59	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	7.522		Crippen Method
mcvol	361.310	ml/mol	McGowan Method
pc	872.22	kPa	Joback Method
rinpol	2810.00		NIST Webbook
rinpol	2810.00		NIST Webbook
tb	954.47	K	Joback Method
tc	1171.23	K	Joback Method
tf	572.07	K	Joback Method
vc	1.437	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1208.38	J/mol×K	954.47	Joback Method
cpg	1225.15	J/mol×K	990.60	Joback Method
cpg	1240.53	J/mol×K	1026.72	Joback Method
cpg	1254.59	J/mol×K	1062.85	Joback Method
cpg	1267.39	J/mol×K	1098.97	Joback Method
cpg	1278.99	J/mol×K	1135.10	Joback Method
cpg	1289.47	J/mol×K	1171.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381643&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