Succinic acid, 8-chlorooctyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C18H22ClF3O4/c19-11-5-3-1-2-4-6-12-25-15(23)9-10-16(24)26-14-8-7-13(20)
InchiKey: AVHUFWSSUQBTAO-UHFFFAOYSA-N
Formula: C18H22ClF3O4
SMILES: O=C(CCC(=O)Oc1ccc(F)c(F)c1F)OCCCCCCCCCCl
Mol. weight [g/mol]: 394.81

Physical Properties

Property code	Value	Unit	Source
gf	-880.00	kJ/mol	Joback Method
hf	-1306.40	kJ/mol	Joback Method
hfus	54.26	kJ/mol	Joback Method
hvap	80.17	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.912		Crippen Method
mcvol	273.150	ml/mol	McGowan Method
pc	1331.98	kPa	Joback Method
rinpol	2526.00		NIST Webbook
rinpol	2526.00		NIST Webbook
tb	840.68	K	Joback Method
tc	1034.83	K	Joback Method
tf	532.61	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.76	J/mol×K	840.68	Joback Method
cpg	822.02	J/mol×K	873.04	Joback Method
cpg	834.31	J/mol×K	905.40	Joback Method
cpg	845.66	J/mol×K	937.76	Joback Method
cpg	856.06	J/mol×K	970.11	Joback Method
cpg	865.53	J/mol×K	1002.47	Joback Method
cpg	874.08	J/mol×K	1034.83	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=U390770&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