Succinic acid, 8-chlorooctyl 3-fluorophenyl ester

Inchi: InChI=1S/C18H24ClFO4/c19-12-5-3-1-2-4-6-13-23-17(21)10-11-18(22)24-16-9-7-8-15(20

InchiKey: UDALJXOXFVKXJH-UHFFFAOYSA-N

Formula: C18H24ClFO4

SMILES: O=C(CCC(=O)Oc1cccc(F)c1)OCCCCCCCCCCl

Mol. weight [g/mol]: 358.83

Physical Properties

Property code	Value	Unit	Source
gf	-471.12	kJ/mol	Joback Method
hf	-891.24	kJ/mol	Joback Method
hfus	48.88	kJ/mol	Joback Method
hvap	80.48	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.634		Crippen Method
mcvol	269.610	ml/mol	McGowan Method
pc	1456.79	kPa	Joback Method
rinpol	2519.00		NIST Webbook
rinpol	2519.00		NIST Webbook
tb	832.18	K	Joback Method
tc	1031.68	K	Joback Method
tf	506.39	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.83	J/mol×K	832.18	Joback Method
cpg	809.93	J/mol×K	865.43	Joback Method
cpg	823.01	J/mol×K	898.68	Joback Method
cpg	835.09	J/mol×K	931.93	Joback Method
cpg	846.19	J/mol×K	965.18	Joback Method
cpg	856.33	J/mol×K	998.43	Joback Method
cpg	865.52	J/mol×K	1031.68	Joback Method

Sources

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=U390338&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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