Succinic acid, 8-chlorooctyl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C19H23ClF4O4/c20-12-5-3-1-2-4-6-13-27-16(25)10-11-17(26)28-15-9-7-8-14(1

InchiKey: SLXIMUQQYNEJOM-UHFFFAOYSA-N

Formula: C19H23ClF4O4

SMILES: O=C(CCC(=O)Oc1cccc(C(F)(F)F)c1F)OCCCCCCCCCl

Mol. weight [g/mol]: 426.83

Physical Properties

Property code	Value	Unit	Source
gf	-1053.92	kJ/mol	Joback Method
hf	-1520.43	kJ/mol	Joback Method
hfus	52.91	kJ/mol	Joback Method
hvap	79.62	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.653		Crippen Method
mcvol	289.010	ml/mol	McGowan Method
pc	1233.74	kPa	Joback Method
rinpol	2531.00		NIST Webbook
tb	854.62	K	Joback Method
tc	1050.16	K	Joback Method
tf	534.37	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.83	J/mol×K	854.62	Joback Method
cpg	889.18	J/mol×K	887.21	Joback Method
cpg	901.54	J/mol×K	919.80	Joback Method
cpg	912.96	J/mol×K	952.39	Joback Method
cpg	923.47	J/mol×K	984.98	Joback Method
cpg	933.09	J/mol×K	1017.57	Joback Method
cpg	941.87	J/mol×K	1050.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390792&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

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