Succinic acid, 8-chlorooctyl pentafluorophenyl ester

Inchi: InChI=1S/C18H20ClF5O4/c19-9-5-3-1-2-4-6-10-27-11(25)7-8-12(26)28-18-16(23)14(21)
InchiKey: JHXUKIHHLXCEOQ-UHFFFAOYSA-N
Formula: C18H20ClF5O4
SMILES: O=C(CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)OCCCCCCCCCCl
Mol. weight [g/mol]: 430.79

Physical Properties

Property code	Value	Unit	Source
gf	-1288.88	kJ/mol	Joback Method
hf	-1721.56	kJ/mol	Joback Method
hfus	59.64	kJ/mol	Joback Method
hvap	79.86	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.190		Crippen Method
mcvol	276.690	ml/mol	McGowan Method
pc	1222.55	kPa	Joback Method
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook
tb	849.18	K	Joback Method
tc	1040.95	K	Joback Method
tf	558.83	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.50	J/mol×K	849.18	Joback Method
cpg	834.13	J/mol×K	881.14	Joback Method
cpg	845.83	J/mol×K	913.10	Joback Method
cpg	856.59	J/mol×K	945.06	Joback Method
cpg	866.41	J/mol×K	977.03	Joback Method
cpg	875.31	J/mol×K	1008.99	Joback Method
cpg	883.28	J/mol×K	1040.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390355&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