Succinic acid, 2,2-dichloroethyl pentafluorobenzyl ester

Inchi: InChI=1S/C13H9Cl2F5O4/c14-6(15)4-24-8(22)2-1-7(21)23-3-5-9(16)11(18)13(20)12(19)
InchiKey: NSLMHBWLDXOZFX-UHFFFAOYSA-N
Formula: C13H9Cl2F5O4
SMILES: O=C(CCC(=O)OCC(Cl)Cl)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 395.11

Physical Properties

Property code	Value	Unit	Source
gf	-1345.35	kJ/mol	Joback Method
hf	-1639.38	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	72.73	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	3.552		Crippen Method
mcvol	218.480	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
tb	771.77	K	Joback Method
tc	961.42	K	Joback Method
tf	517.40	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.48	J/mol×K	771.77	Joback Method
cpg	579.99	J/mol×K	803.38	Joback Method
cpg	588.82	J/mol×K	834.99	Joback Method
cpg	596.98	J/mol×K	866.59	Joback Method
cpg	604.45	J/mol×K	898.20	Joback Method
cpg	611.23	J/mol×K	929.81	Joback Method
cpg	617.30	J/mol×K	961.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389882&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