Succinic acid, 2,2,3,3-tetrafluoropropyl 3-chlorophenyl ester

Inchi: InChI=1S/C13H11ClF4O4/c14-8-2-1-3-9(6-8)22-11(20)5-4-10(19)21-7-13(17,18)12(15)16

InchiKey: VMYUTFJYILVOGE-UHFFFAOYSA-N

Formula: C13H11ClF4O4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 342.67

Physical Properties

Property code	Value	Unit	Source
gf	-1097.25	kJ/mol	Joback Method
hf	-1390.40	kJ/mol	Joback Method
hfus	34.23	kJ/mol	Joback Method
hvap	65.22	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.469		Crippen Method
mcvol	204.470	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1837.00		NIST Webbook
rinpol	1837.00		NIST Webbook
tb	711.92	K	Joback Method
tc	906.27	K	Joback Method
tf	439.23	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.03	J/mol×K	711.92	Joback Method
cpg	559.31	J/mol×K	744.31	Joback Method
cpg	569.77	J/mol×K	776.70	Joback Method
cpg	579.46	J/mol×K	809.10	Joback Method
cpg	588.40	J/mol×K	841.49	Joback Method
cpg	596.60	J/mol×K	873.88	Joback Method
cpg	604.10	J/mol×K	906.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389846&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