Succinic acid, 2,2,3,3-tetrafluoropropyl 2-chloro-4-methylphenyl ester

Inchi: InChI=1S/C14H13ClF4O4/c1-8-2-3-10(9(15)6-8)23-12(21)5-4-11(20)22-7-14(18,19)13(16

InchiKey: BNBFPHXNJYILJR-UHFFFAOYSA-N

Formula: C14H13ClF4O4

SMILES: Cc1ccc(OC(=O)CCC(=O)OCC(F)(F)C(F)F)c(Cl)c1

Mol. weight [g/mol]: 356.70

Physical Properties

Property code	Value	Unit	Source
gf	-1098.46	kJ/mol	Joback Method
hf	-1422.51	kJ/mol	Joback Method
hfus	36.43	kJ/mol	Joback Method
hvap	68.10	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.778		Crippen Method
mcvol	218.560	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	1912.00		NIST Webbook
rinpol	1912.00		NIST Webbook
tb	739.78	K	Joback Method
tc	933.73	K	Joback Method
tf	463.02	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.10	J/mol×K	739.78	Joback Method
cpg	610.70	J/mol×K	772.11	Joback Method
cpg	621.49	J/mol×K	804.43	Joback Method
cpg	631.49	J/mol×K	836.76	Joback Method
cpg	640.71	J/mol×K	869.08	Joback Method
cpg	649.18	J/mol×K	901.41	Joback Method
cpg	656.92	J/mol×K	933.73	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=U390209&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