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

Inchi: InChI=1S/C14H12ClF5O4/c1-8-6-9(2-3-10(8)15)24-12(22)5-4-11(21)23-7-13(16,17)14(18

InchiKey: HUQZOAINGHJAEL-UHFFFAOYSA-N

Formula: C14H12ClF5O4

SMILES: Cc1cc(OC(=O)CCC(=O)OCC(F)(F)C(F)(F)F)ccc1Cl

Mol. weight [g/mol]: 374.69

Physical Properties

Property code	Value	Unit	Source
gf	-1287.99	kJ/mol	Joback Method
hf	-1622.09	kJ/mol	Joback Method
hfus	35.62	kJ/mol	Joback Method
hvap	66.38	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.075		Crippen Method
mcvol	220.330	ml/mol	McGowan Method
pc	1746.28	kPa	Joback Method
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
tb	736.26	K	Joback Method
tc	928.78	K	Joback Method
tf	481.03	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.90	J/mol×K	736.26	Joback Method
cpg	620.05	J/mol×K	768.35	Joback Method
cpg	630.39	J/mol×K	800.43	Joback Method
cpg	639.95	J/mol×K	832.52	Joback Method
cpg	648.76	J/mol×K	864.61	Joback Method
cpg	656.87	J/mol×K	896.69	Joback Method
cpg	664.30	J/mol×K	928.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390873&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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