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

Inchi: InChI=1S/C14H13ClF4O5/c1-22-10-6-8(15)2-3-9(10)24-12(21)5-4-11(20)23-7-14(18,19)1

InchiKey: QKHIVTCHMIHRJM-UHFFFAOYSA-N

Formula: C14H13ClF4O5

SMILES: COc1cc(Cl)ccc1OC(=O)CCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 372.70

Physical Properties

Property code	Value	Unit	Source
gf	-1203.46	kJ/mol	Joback Method
hf	-1554.73	kJ/mol	Joback Method
hfus	37.62	kJ/mol	Joback Method
hvap	70.51	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.478		Crippen Method
mcvol	224.430	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
tb	762.20	K	Joback Method
tc	956.02	K	Joback Method
tf	485.25	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.78	J/mol×K	762.20	Joback Method
cpg	636.14	J/mol×K	794.50	Joback Method
cpg	646.65	J/mol×K	826.81	Joback Method
cpg	656.33	J/mol×K	859.11	Joback Method
cpg	665.19	J/mol×K	891.41	Joback Method
cpg	673.24	J/mol×K	923.72	Joback Method
cpg	680.49	J/mol×K	956.02	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390929&Units=SI

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