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

Inchi: InChI=1S/C15H16F4O4/c1-9-4-3-5-11(10(9)2)23-13(21)7-6-12(20)22-8-15(18,19)14(16)1

InchiKey: FZJAIKLQOFPTCY-UHFFFAOYSA-N

Formula: C15H16F4O4

SMILES: Cc1cccc(OC(=O)CCC(=O)OCC(F)(F)C(F)F)c1C

Mol. weight [g/mol]: 336.28

Physical Properties

Property code	Value	Unit	Source
gf	-1078.11	kJ/mol	Joback Method
hf	-1427.41	kJ/mol	Joback Method
hfus	34.83	kJ/mol	Joback Method
hvap	65.94	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.433		Crippen Method
mcvol	220.410	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	1859.00		NIST Webbook
rinpol	1859.00		NIST Webbook
tb	725.23	K	Joback Method
tc	914.08	K	Joback Method
tf	444.37	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.01	J/mol×K	725.23	Joback Method
cpg	640.02	J/mol×K	756.71	Joback Method
cpg	652.20	J/mol×K	788.18	Joback Method
cpg	663.56	J/mol×K	819.66	Joback Method
cpg	674.13	J/mol×K	851.13	Joback Method
cpg	683.91	J/mol×K	882.61	Joback Method
cpg	692.94	J/mol×K	914.08	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=U390013&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