Succinic acid, 2,2,3,3-tetrafluoropropyl 1-phenylpropyl ester

Inchi: InChI=1S/C16H18F4O4/c1-2-12(11-6-4-3-5-7-11)24-14(22)9-8-13(21)23-10-16(19,20)15

InchiKey: RGPKYNWFVQSGRZ-UHFFFAOYSA-N

Formula: C16H18F4O4

SMILES: CCC(OC(=O)CCC(=O)OCC(F)(F)C(F)F)c1ccccc1

Mol. weight [g/mol]: 350.31

Physical Properties

Property code	Value	Unit	Source
gf	-1052.87	kJ/mol	Joback Method
hf	-1430.39	kJ/mol	Joback Method
hfus	34.67	kJ/mol	Joback Method
hvap	66.46	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.905		Crippen Method
mcvol	234.500	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpol	1801.00		NIST Webbook
rinpol	1801.00		NIST Webbook
tb	737.71	K	Joback Method
tc	926.69	K	Joback Method
tf	415.60	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.54	J/mol×K	737.71	Joback Method
cpg	697.34	J/mol×K	769.21	Joback Method
cpg	710.21	J/mol×K	800.70	Joback Method
cpg	722.18	J/mol×K	832.20	Joback Method
cpg	733.29	J/mol×K	863.70	Joback Method
cpg	743.56	J/mol×K	895.19	Joback Method
cpg	753.02	J/mol×K	926.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389920&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