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

Inchi: InChI=1S/C13H11F5O4/c14-8-2-1-3-9(6-8)22-11(20)5-4-10(19)21-7-13(17,18)12(15)16/h

InchiKey: SHMVTGBRZYXLHV-UHFFFAOYSA-N

Formula: C13H11F5O4

SMILES: O=C(CCC(=O)Oc1cccc(F)c1)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 326.22

Physical Properties

Property code	Value	Unit	Source
gf	-1280.13	kJ/mol	Joback Method
hf	-1570.77	kJ/mol	Joback Method
hfus	33.11	kJ/mol	Joback Method
hvap	60.01	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.955		Crippen Method
mcvol	194.000	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	1636.00		NIST Webbook
rinpol	1636.00		NIST Webbook
tb	673.76	K	Joback Method
tc	857.46	K	Joback Method
tf	409.90	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.03	J/mol×K	673.76	Joback Method
cpg	542.81	J/mol×K	704.38	Joback Method
cpg	553.83	J/mol×K	734.99	Joback Method
cpg	564.13	J/mol×K	765.61	Joback Method
cpg	573.71	J/mol×K	796.23	Joback Method
cpg	582.60	J/mol×K	826.85	Joback Method
cpg	590.82	J/mol×K	857.46	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=U390323&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