Succinic acid, 2,2,3,3-tetrafluoropropyl trans-4-methylcyclohexyl ester

Inchi: InChI=1S/C14H20F4O4/c1-9-2-4-10(5-3-9)22-12(20)7-6-11(19)21-8-14(17,18)13(15)16/h

InchiKey: VYKIQYFLEARILO-UHFFFAOYSA-N

Formula: C14H20F4O4

SMILES: CC1CCC(OC(=O)CCC(=O)OCC(F)(F)C(F)F)CC1

Mol. weight [g/mol]: 328.30

Physical Properties

Property code	Value	Unit	Source
gf	-1162.94	kJ/mol	Joback Method
hf	-1586.38	kJ/mol	Joback Method
hfus	31.88	kJ/mol	Joback Method
hvap	60.24	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.332		Crippen Method
mcvol	219.220	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
tb	680.59	K	Joback Method
tc	863.87	K	Joback Method
tf	384.78	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.43	J/mol×K	680.59	Joback Method
cpg	668.90	J/mol×K	711.14	Joback Method
cpg	684.39	J/mol×K	741.68	Joback Method
cpg	698.92	J/mol×K	772.23	Joback Method
cpg	712.51	J/mol×K	802.78	Joback Method
cpg	725.16	J/mol×K	833.32	Joback Method
cpg	736.91	J/mol×K	863.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390066&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