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

Inchi: InChI=1S/C12H16F4O4/c13-11(14)12(15,16)7-19-9(17)5-6-10(18)20-8-3-1-2-4-8/h8,11H

InchiKey: JEMHMPXMXVVNOB-UHFFFAOYSA-N

Formula: C12H16F4O4

SMILES: O=C(CCC(=O)OC1CCCC1)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 300.25

Physical Properties

Property code	Value	Unit	Source
gf	-1159.97	kJ/mol	Joback Method
hf	-1518.60	kJ/mol	Joback Method
hfus	27.73	kJ/mol	Joback Method
hvap	55.92	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.696		Crippen Method
mcvol	191.040	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	1530.00		NIST Webbook
rinpol	1530.00		NIST Webbook
tb	635.23	K	Joback Method
tc	816.29	K	Joback Method
tf	370.00	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.97	J/mol×K	635.23	Joback Method
cpg	555.66	J/mol×K	665.41	Joback Method
cpg	569.51	J/mol×K	695.58	Joback Method
cpg	582.53	J/mol×K	725.76	Joback Method
cpg	594.75	J/mol×K	755.93	Joback Method
cpg	606.20	J/mol×K	786.11	Joback Method
cpg	616.89	J/mol×K	816.29	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=U391371&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