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

Inchi: InChI=1S/C14H22F4O4/c1-3-5-6-10(4-2)22-12(20)8-7-11(19)21-9-14(17,18)13(15)16/h1

InchiKey: JQHOLXMHKPIRDD-UHFFFAOYSA-N

Formula: C14H22F4O4

SMILES: CCCCC(CC)OC(=O)CCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 330.32

Physical Properties

Property code	Value	Unit	Source
gf	-1182.12	kJ/mol	Joback Method
hf	-1625.64	kJ/mol	Joback Method
hfus	35.45	kJ/mol	Joback Method
hvap	59.73	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.722		Crippen Method
mcvol	230.080	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	1542.00		NIST Webbook
rinpol	1542.00		NIST Webbook
tb	665.27	K	Joback Method
tc	831.28	K	Joback Method
tf	366.64	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.37	J/mol×K	665.27	Joback Method
cpg	671.83	J/mol×K	692.94	Joback Method
cpg	685.58	J/mol×K	720.61	Joback Method
cpg	698.62	J/mol×K	748.28	Joback Method
cpg	710.96	J/mol×K	775.94	Joback Method
cpg	722.64	J/mol×K	803.61	Joback Method
cpg	733.66	J/mol×K	831.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390595&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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