Succinic acid, hept-2-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C14H21F5O4/c1-3-4-5-6-10(2)23-12(21)8-7-11(20)22-9-13(15,16)14(17,18)19/

InchiKey: WIDJGMOXZBCZRL-UHFFFAOYSA-N

Formula: C14H21F5O4

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

Mol. weight [g/mol]: 348.31

Physical Properties

Property code	Value	Unit	Source
gf	-1371.65	kJ/mol	Joback Method
hf	-1825.22	kJ/mol	Joback Method
hfus	34.64	kJ/mol	Joback Method
hvap	58.01	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.019		Crippen Method
mcvol	231.850	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
tb	661.75	K	Joback Method
tc	826.51	K	Joback Method
tf	384.65	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.52	J/mol×K	661.75	Joback Method
cpg	681.65	J/mol×K	689.21	Joback Method
cpg	695.04	J/mol×K	716.67	Joback Method
cpg	707.71	J/mol×K	744.13	Joback Method
cpg	719.68	J/mol×K	771.59	Joback Method
cpg	730.97	J/mol×K	799.05	Joback Method
cpg	741.62	J/mol×K	826.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390866&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