Succinic acid, 1,1,1-trifluoroprop-2-yl 2-heptyl ester

Inchi: InChI=1S/C14H23F3O4/c1-4-5-6-7-10(2)20-12(18)8-9-13(19)21-11(3)14(15,16)17/h10-1

InchiKey: HSTLIYSPZHMCMA-UHFFFAOYSA-N

Formula: C14H23F3O4

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

Mol. weight [g/mol]: 312.33

Physical Properties

Property code	Value	Unit	Source
gf	-987.31	kJ/mol	Joback Method
hf	-1429.53	kJ/mol	Joback Method
hfus	32.37	kJ/mol	Joback Method
hvap	60.55	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.773		Crippen Method
mcvol	228.310	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	1487.00		NIST Webbook
rinpol	1487.00		NIST Webbook
tb	666.00	K	Joback Method
tc	836.73	K	Joback Method
tf	366.05	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.44	J/mol×K	666.00	Joback Method
cpg	664.37	J/mol×K	694.46	Joback Method
cpg	678.54	J/mol×K	722.91	Joback Method
cpg	691.97	J/mol×K	751.37	Joback Method
cpg	704.68	J/mol×K	779.82	Joback Method
cpg	716.69	J/mol×K	808.28	Joback Method
cpg	728.00	J/mol×K	836.73	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=U390564&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