Succinic acid, 1,1,1-trifluoro-2-propyl 3-pentyl ester

Inchi: InChI=1S/C12H19F3O4/c1-4-9(5-2)19-11(17)7-6-10(16)18-8(3)12(13,14)15/h8-9H,4-7H2

InchiKey: AGZAFEUKLZXKMX-UHFFFAOYSA-N

Formula: C12H19F3O4

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

Mol. weight [g/mol]: 284.27

Physical Properties

Property code	Value	Unit	Source
gf	-1004.15	kJ/mol	Joback Method
hf	-1388.25	kJ/mol	Joback Method
hfus	27.19	kJ/mol	Joback Method
hvap	56.09	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.992		Crippen Method
mcvol	200.130	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	1293.00		NIST Webbook
tb	620.24	K	Joback Method
tc	791.52	K	Joback Method
tf	343.51	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.97	J/mol×K	620.24	Joback Method
cpg	557.89	J/mol×K	648.79	Joback Method
cpg	571.12	J/mol×K	677.33	Joback Method
cpg	583.69	J/mol×K	705.88	Joback Method
cpg	595.59	J/mol×K	734.42	Joback Method
cpg	606.86	J/mol×K	762.97	Joback Method
cpg	617.49	J/mol×K	791.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370912&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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