Succinic acid, 1,1,1-trifluoroprop-2-yl pent-4-en-2-yl ester

Inchi: InChI=1S/C12H17F3O4/c1-4-5-8(2)18-10(16)6-7-11(17)19-9(3)12(13,14)15/h4,8-9H,1,5-

InchiKey: VWGKDENEBJFXMW-UHFFFAOYSA-N

Formula: C12H17F3O4

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

Mol. weight [g/mol]: 282.26

Physical Properties

Property code	Value	Unit	Source
gf	-916.31	kJ/mol	Joback Method
hf	-1262.82	kJ/mol	Joback Method
hfus	25.91	kJ/mol	Joback Method
hvap	55.42	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.768		Crippen Method
mcvol	195.830	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1310.00		NIST Webbook
rinpol	1310.00		NIST Webbook
tb	616.92	K	Joback Method
tc	790.59	K	Joback Method
tf	341.75	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.33	J/mol×K	616.92	Joback Method
cpg	535.71	J/mol×K	645.87	Joback Method
cpg	548.40	J/mol×K	674.81	Joback Method
cpg	560.42	J/mol×K	703.76	Joback Method
cpg	571.78	J/mol×K	732.70	Joback Method
cpg	582.51	J/mol×K	761.65	Joback Method
cpg	592.62	J/mol×K	790.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391149&Units=SI

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