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

Inchi: InChI=1S/C12H17F3O5/c1-8(12(13,14)15)20-11(17)5-4-10(16)19-7-9-3-2-6-18-9/h8-9H,2

InchiKey: ROFPXNSZHQLGJT-UHFFFAOYSA-N

Formula: C12H17F3O5

SMILES: CC(OC(=O)CCC(=O)OCC1CCCO1)C(F)(F)F

Mol. weight [g/mol]: 298.26

Physical Properties

Property code	Value	Unit	Source
gf	-1051.28	kJ/mol	Joback Method
hf	-1454.49	kJ/mol	Joback Method
hfus	32.63	kJ/mol	Joback Method
hvap	61.25	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.983		Crippen Method
mcvol	195.140	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1578.00		NIST Webbook
rinpol	1578.00		NIST Webbook
tb	662.91	K	Joback Method
tc	850.66	K	Joback Method
tf	395.98	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.06	J/mol×K	662.91	Joback Method
cpg	579.68	J/mol×K	694.20	Joback Method
cpg	593.42	J/mol×K	725.49	Joback Method
cpg	606.29	J/mol×K	756.79	Joback Method
cpg	618.32	J/mol×K	788.08	Joback Method
cpg	629.54	J/mol×K	819.37	Joback Method
cpg	639.97	J/mol×K	850.66	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=U390710&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