Succinic acid, 1,1,1-trifluoroprop-2-yl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C12H11F11O4/c1-5(11(19,20)21)27-7(25)3-2-6(24)26-4-9(15,16)12(22,23)10(

InchiKey: KJNKITVQHMRYRU-UHFFFAOYSA-N

Formula: C12H11F11O4

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

Mol. weight [g/mol]: 428.20

Physical Properties

Property code	Value	Unit	Source
gf	-2554.11	kJ/mol	Joback Method
hf	-2983.38	kJ/mol	Joback Method
hfus	29.59	kJ/mol	Joback Method
hvap	45.67	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.975		Crippen Method
mcvol	214.290	ml/mol	McGowan Method
pc	1391.25	kPa	Joback Method
rinpol	1237.00		NIST Webbook
tb	604.71	K	Joback Method
tc	753.71	K	Joback Method
tf	355.49	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.85	J/mol×K	604.71	Joback Method
cpg	629.61	J/mol×K	629.54	Joback Method
cpg	640.66	J/mol×K	654.38	Joback Method
cpg	651.03	J/mol×K	679.21	Joback Method
cpg	660.75	J/mol×K	704.04	Joback Method
cpg	669.85	J/mol×K	728.88	Joback Method
cpg	678.37	J/mol×K	753.71	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=U390699&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