Succinic acid, tridec-2-yn-1-yl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C21H30F6O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-30-17(28)13-14-18(29)31-16-20
InchiKey: BYGXEVXWLBIJSL-UHFFFAOYSA-N
Formula: C21H30F6O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCC(=O)OCC(F)(F)C(F)C(F)(F)F
Mol. weight [g/mol]: 460.45

Physical Properties

Property code	Value	Unit	Source
gf	-1304.72	kJ/mol	Joback Method
hf	-1893.51	kJ/mol	Joback Method
hfus	58.97	kJ/mol	Joback Method
hvap	74.92	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	5.923		Crippen Method
mcvol	323.650	ml/mol	McGowan Method
pc	972.91	kPa	Joback Method
rinpol	2293.00		NIST Webbook
rinpol	2293.00		NIST Webbook
tb	830.18	K	Joback Method
tc	1016.57	K	Joback Method
tf	570.23	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1026.36	J/mol×K	830.18	Joback Method
cpg	1042.42	J/mol×K	861.25	Joback Method
cpg	1057.48	J/mol×K	892.31	Joback Method
cpg	1071.58	J/mol×K	923.38	Joback Method
cpg	1084.77	J/mol×K	954.44	Joback Method
cpg	1097.09	J/mol×K	985.51	Joback Method
cpg	1108.59	J/mol×K	1016.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390815&Units=SI
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

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