Succinic acid, hex-4-yn-3-yl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C13H16F4O4/c1-3-5-9(4-2)21-11(19)7-6-10(18)20-8-13(16,17)12(14)15/h9,12H

InchiKey: MWGANCKJNQZBOW-UHFFFAOYSA-N

Formula: C13H16F4O4

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

Mol. weight [g/mol]: 312.26

Physical Properties

Property code	Value	Unit	Source
gf	-987.74	kJ/mol	Joback Method
hf	-1332.70	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	59.66	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.555		Crippen Method
mcvol	207.390	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	1548.00		NIST Webbook
rinpol	1548.00		NIST Webbook
tb	651.39	K	Joback Method
tc	830.88	K	Joback Method
tf	461.47	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.92	J/mol×K	651.39	Joback Method
cpg	575.13	J/mol×K	681.31	Joback Method
cpg	587.63	J/mol×K	711.22	Joback Method
cpg	599.44	J/mol×K	741.14	Joback Method
cpg	610.57	J/mol×K	771.05	Joback Method
cpg	621.04	J/mol×K	800.97	Joback Method
cpg	630.85	J/mol×K	830.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390851&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

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