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

Inchi: InChI=1S/C13H15F5O4/c1-3-5-9(4-2)22-11(20)7-6-10(19)21-8-12(14,15)13(16,17)18/h9

InchiKey: SHWZAPYHGJSQPL-UHFFFAOYSA-N

Formula: C13H15F5O4

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

Mol. weight [g/mol]: 330.25

Physical Properties

Property code	Value	Unit	Source
gf	-1177.27	kJ/mol	Joback Method
hf	-1532.28	kJ/mol	Joback Method
hfus	35.17	kJ/mol	Joback Method
hvap	57.93	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.853		Crippen Method
mcvol	209.160	ml/mol	McGowan Method
pc	1746.28	kPa	Joback Method
rinpol	1412.00		NIST Webbook
tb	647.87	K	Joback Method
tc	825.86	K	Joback Method
tf	479.48	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.50	J/mol×K	647.87	Joback Method
cpg	585.37	J/mol×K	677.54	Joback Method
cpg	597.50	J/mol×K	707.20	Joback Method
cpg	608.90	J/mol×K	736.87	Joback Method
cpg	619.62	J/mol×K	766.53	Joback Method
cpg	629.67	J/mol×K	796.20	Joback Method
cpg	639.07	J/mol×K	825.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390865&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