Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl non-5-yn-3-yl ester

Inchi: InChI=1S/C18H22F8O4/c1-3-5-6-7-8-12(4-2)30-14(28)10-9-13(27)29-11-16(21,22)18(25

InchiKey: QSUYVFGVAZTKLT-UHFFFAOYSA-N

Formula: C18H22F8O4

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

Mol. weight [g/mol]: 454.35

Physical Properties

Property code	Value	Unit	Source
gf	-1719.20	kJ/mol	Joback Method
hf	-2237.84	kJ/mol	Joback Method
hfus	46.42	kJ/mol	Joback Method
hvap	64.93	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	4.996		Crippen Method
mcvol	284.920	ml/mol	McGowan Method
pc	1125.32	kPa	Joback Method
rinpol	1858.00		NIST Webbook
rinpol	1858.00		NIST Webbook
tb	756.41	K	Joback Method
tc	931.13	K	Joback Method
tf	525.02	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.32	J/mol×K	756.41	Joback Method
cpg	883.50	J/mol×K	785.53	Joback Method
cpg	896.80	J/mol×K	814.65	Joback Method
cpg	909.27	J/mol×K	843.77	Joback Method
cpg	920.95	J/mol×K	872.89	Joback Method
cpg	931.90	J/mol×K	902.01	Joback Method
cpg	942.15	J/mol×K	931.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391007&Units=SI

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