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

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

InchiKey: DYTFJSUGGHDNBL-UHFFFAOYSA-N

Formula: C18H22F8O4

SMILES: CCC#CC(CC(C)C)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	-1721.64	kJ/mol	Joback Method
hf	-2243.12	kJ/mol	Joback Method
hfus	42.90	kJ/mol	Joback Method
hvap	64.54	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.852		Crippen Method
mcvol	284.920	ml/mol	McGowan Method
pc	1131.38	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
tb	755.97	K	Joback Method
tc	931.77	K	Joback Method
tf	510.02	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.85	J/mol×K	755.97	Joback Method
cpg	884.13	J/mol×K	785.27	Joback Method
cpg	897.51	J/mol×K	814.57	Joback Method
cpg	910.04	J/mol×K	843.87	Joback Method
cpg	921.77	J/mol×K	873.17	Joback Method
cpg	932.75	J/mol×K	902.47	Joback Method
cpg	943.02	J/mol×K	931.77	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=U391024&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