Succinic acid, 2,2,3,3-tetrafluoropropyl 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C18H24F4O4/c1-5-6-13(4)14(8-7-12(2)3)26-16(24)10-9-15(23)25-11-18(21,22

InchiKey: CTKSPNSBWPLIQV-UHFFFAOYSA-N

Formula: C18H24F4O4

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

Mol. weight [g/mol]: 380.37

Physical Properties

Property code	Value	Unit	Source
gf	-868.79	kJ/mol	Joback Method
hf	-1325.54	kJ/mol	Joback Method
hfus	42.82	kJ/mol	Joback Method
hvap	69.81	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.138		Crippen Method
mcvol	273.540	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	1815.00		NIST Webbook
rinpol	1815.00		NIST Webbook
tb	761.91	K	Joback Method
tc	946.51	K	Joback Method
tf	487.10	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.64	J/mol×K	761.91	Joback Method
cpg	824.77	J/mol×K	792.68	Joback Method
cpg	839.00	J/mol×K	823.44	Joback Method
cpg	852.34	J/mol×K	854.21	Joback Method
cpg	864.83	J/mol×K	884.98	Joback Method
cpg	876.49	J/mol×K	915.74	Joback Method
cpg	887.36	J/mol×K	946.51	Joback Method

Sources

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=U391015&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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