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

Inchi: InChI=1S/C18H25F3O4/c1-6-7-13(4)15(9-8-12(2)3)25-17(23)11-10-16(22)24-14(5)18(19

InchiKey: SBKKZCMYUZLGFC-UHFFFAOYSA-N

Formula: C18H25F3O4

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

Mol. weight [g/mol]: 362.38

Physical Properties

Property code	Value	Unit	Source
gf	-673.98	kJ/mol	Joback Method
hf	-1129.43	kJ/mol	Joback Method
hfus	39.74	kJ/mol	Joback Method
hvap	70.62	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.188		Crippen Method
mcvol	271.770	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
tb	762.64	K	Joback Method
tc	951.81	K	Joback Method
tf	486.51	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.99	J/mol×K	762.64	Joback Method
cpg	817.58	J/mol×K	794.17	Joback Method
cpg	832.21	J/mol×K	825.70	Joback Method
cpg	845.93	J/mol×K	857.22	Joback Method
cpg	858.76	J/mol×K	888.75	Joback Method
cpg	870.74	J/mol×K	920.28	Joback Method
cpg	881.88	J/mol×K	951.81	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=U391014&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