Succinic acid, 2-fluorophenyl non-5-yn-3-yl ester

Inchi: InChI=1S/C19H23FO4/c1-3-5-6-7-10-15(4-2)23-18(21)13-14-19(22)24-17-12-9-8-11-16(1

InchiKey: NKQHOWHWFULFNW-UHFFFAOYSA-N

Formula: C19H23FO4

SMILES: CCCC#CCC(CC)OC(=O)CCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 334.38

Physical Properties

Property code	Value	Unit	Source
gf	-250.41	kJ/mol	Joback Method
hf	-629.12	kJ/mol	Joback Method
hfus	46.87	kJ/mol	Joback Method
hvap	80.09	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.027		Crippen Method
mcvol	262.860	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2290.00		NIST Webbook
rinpol	2290.00		NIST Webbook
tb	826.19	K	Joback Method
tc	1035.78	K	Joback Method
tf	578.84	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.27	J/mol×K	826.19	Joback Method
cpg	791.16	J/mol×K	861.12	Joback Method
cpg	804.93	J/mol×K	896.05	Joback Method
cpg	817.61	J/mol×K	930.98	Joback Method
cpg	829.22	J/mol×K	965.92	Joback Method
cpg	839.76	J/mol×K	1000.85	Joback Method
cpg	849.26	J/mol×K	1035.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391012&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