Succinic acid, hex-4-yn-3-yl 3-fluorophenyl ester

Inchi: InChI=1S/C16H17FO4/c1-3-6-13(4-2)20-15(18)9-10-16(19)21-14-8-5-7-12(17)11-14/h5,7

InchiKey: RXGDSFBAZQEQQX-UHFFFAOYSA-N

Formula: C16H17FO4

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 292.30

Physical Properties

Property code	Value	Unit	Source
gf	-275.67	kJ/mol	Joback Method
hf	-567.20	kJ/mol	Joback Method
hfus	39.10	kJ/mol	Joback Method
hvap	73.41	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	2.856		Crippen Method
mcvol	220.590	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook
tb	757.55	K	Joback Method
tc	972.79	K	Joback Method
tf	545.03	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.67	J/mol×K	757.55	Joback Method
cpg	622.79	J/mol×K	793.42	Joback Method
cpg	635.90	J/mol×K	829.30	Joback Method
cpg	648.00	J/mol×K	865.17	Joback Method
cpg	659.12	J/mol×K	901.04	Joback Method
cpg	669.26	J/mol×K	936.91	Joback Method
cpg	678.43	J/mol×K	972.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390330&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