Succinic acid, hex-4-yn-3-yl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C17H19FO5/c1-4-6-13(5-2)22-16(19)9-10-17(20)23-14-8-7-12(18)11-15(14)21

InchiKey: QDNMRAIIJURBJL-UHFFFAOYSA-N

Formula: C17H19FO5

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 322.33

Physical Properties

Property code	Value	Unit	Source
gf	-381.88	kJ/mol	Joback Method
hf	-731.53	kJ/mol	Joback Method
hfus	42.49	kJ/mol	Joback Method
hvap	78.70	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	2.865		Crippen Method
mcvol	240.550	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	2202.00		NIST Webbook
rinpol	2202.00		NIST Webbook
tb	807.83	K	Joback Method
tc	1020.23	K	Joback Method
tf	591.05	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.64	J/mol×K	807.83	Joback Method
cpg	703.53	J/mol×K	843.23	Joback Method
cpg	716.32	J/mol×K	878.63	Joback Method
cpg	728.02	J/mol×K	914.03	Joback Method
cpg	738.61	J/mol×K	949.43	Joback Method
cpg	748.08	J/mol×K	984.83	Joback Method
cpg	756.43	J/mol×K	1020.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390902&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

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