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

Inchi: InChI=1S/C15H15FO5/c1-4-10(2)20-14(17)7-8-15(18)21-12-6-5-11(16)9-13(12)19-3/h1,5

InchiKey: DMOSNKLAPQKIGI-UHFFFAOYSA-N

Formula: C15H15FO5

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

Mol. weight [g/mol]: 294.27

Physical Properties

Property code	Value	Unit	Source
gf	-378.45	kJ/mol	Joback Method
hf	-670.65	kJ/mol	Joback Method
hfus	37.16	kJ/mol	Joback Method
hvap	71.96	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.085		Crippen Method
mcvol	212.370	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	1991.00		NIST Webbook
rinpol	1991.00		NIST Webbook
tb	743.19	K	Joback Method
tc	952.13	K	Joback Method
tf	509.38	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.72	J/mol×K	743.19	Joback Method
cpg	590.70	J/mol×K	778.01	Joback Method
cpg	602.77	J/mol×K	812.84	Joback Method
cpg	613.94	J/mol×K	847.66	Joback Method
cpg	624.20	J/mol×K	882.48	Joback Method
cpg	633.55	J/mol×K	917.31	Joback Method
cpg	641.97	J/mol×K	952.13	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=U390897&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