Succinic acid, but-3-yn-2-yl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C15H12F4O4/c1-3-9(2)22-12(20)7-8-13(21)23-11-6-4-5-10(14(11)16)15(17,18

InchiKey: DFWZTBXBZXFMEI-UHFFFAOYSA-N

Formula: C15H12F4O4

SMILES: C#CC(C)OC(=O)CCC(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 332.25

Physical Properties

Property code	Value	Unit	Source
gf	-855.04	kJ/mol	Joback Method
hf	-1135.51	kJ/mol	Joback Method
hfus	37.80	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.095		Crippen Method
mcvol	211.810	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1753.00		NIST Webbook
tb	715.35	K	Joback Method
tc	912.51	K	Joback Method
tf	491.34	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.15	J/mol×K	715.35	Joback Method
cpg	590.08	J/mol×K	748.21	Joback Method
cpg	601.19	J/mol×K	781.07	Joback Method
cpg	611.50	J/mol×K	813.93	Joback Method
cpg	621.05	J/mol×K	846.79	Joback Method
cpg	629.86	J/mol×K	879.65	Joback Method
cpg	637.95	J/mol×K	912.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390779&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