Succinic acid, but-3-yn-2-yl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C14H12BrFO4/c1-3-9(2)19-13(17)6-7-14(18)20-12-5-4-10(16)8-11(12)15/h1,4-

InchiKey: YPOQEMYXQHZJKO-UHFFFAOYSA-N

Formula: C14H12BrFO4

SMILES: C#CC(C)OC(=O)CCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 343.14

Physical Properties

Property code	Value	Unit	Source
gf	-267.55	kJ/mol	Joback Method
hf	-491.46	kJ/mol	Joback Method
hfus	38.67	kJ/mol	Joback Method
hvap	73.76	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	2.839		Crippen Method
mcvol	209.910	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1976.00		NIST Webbook
rinpol	1976.00		NIST Webbook
tb	764.05	K	Joback Method
tc	987.73	K	Joback Method
tf	535.68	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.70	J/mol×K	764.05	Joback Method
cpg	545.03	J/mol×K	801.33	Joback Method
cpg	555.47	J/mol×K	838.61	Joback Method
cpg	565.06	J/mol×K	875.89	Joback Method
cpg	573.81	J/mol×K	913.17	Joback Method
cpg	581.73	J/mol×K	950.45	Joback Method
cpg	588.86	J/mol×K	987.73	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389763&Units=SI

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