Succinic acid, but-3-yn-2-yl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C16H18O4/c1-5-12(3)19-15(17)9-10-16(18)20-14-8-6-7-11(2)13(14)4/h1,6-8,1

InchiKey: VAVKTOJIXWXKDO-UHFFFAOYSA-N

Formula: C16H18O4

SMILES: C#CC(C)OC(=O)CCC(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 274.31

Physical Properties

Property code	Value	Unit	Source
gf	-70.22	kJ/mol	Joback Method
hf	-362.96	kJ/mol	Joback Method
hfus	35.49	kJ/mol	Joback Method
hvap	72.59	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	2.554		Crippen Method
mcvol	218.820	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook
tb	744.38	K	Joback Method
tc	960.36	K	Joback Method
tf	497.83	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.32	J/mol×K	744.38	Joback Method
cpg	611.61	J/mol×K	780.38	Joback Method
cpg	624.92	J/mol×K	816.37	Joback Method
cpg	637.27	J/mol×K	852.37	Joback Method
cpg	648.67	J/mol×K	888.36	Joback Method
cpg	659.12	J/mol×K	924.36	Joback Method
cpg	668.64	J/mol×K	960.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390015&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