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

Inchi: InChI=1S/C15H16O5/c1-4-11(2)19-14(16)9-10-15(17)20-13-8-6-5-7-12(13)18-3/h1,5-8,1

InchiKey: VHAPNBSNNMBLQZ-UHFFFAOYSA-N

Formula: C15H16O5

SMILES: C#CC(C)OC(=O)CCC(=O)Oc1ccccc1OC

Mol. weight [g/mol]: 276.28

Physical Properties

Property code	Value	Unit	Source
gf	-174.01	kJ/mol	Joback Method
hf	-463.07	kJ/mol	Joback Method
hfus	34.47	kJ/mol	Joback Method
hvap	72.11	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	1.946		Crippen Method
mcvol	210.600	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1984.00		NIST Webbook
rinpol	1984.00		NIST Webbook
tb	738.94	K	Joback Method
tc	955.06	K	Joback Method
tf	496.27	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.07	J/mol×K	738.94	Joback Method
cpg	584.74	J/mol×K	774.96	Joback Method
cpg	597.44	J/mol×K	810.98	Joback Method
cpg	609.15	J/mol×K	847.00	Joback Method
cpg	619.89	J/mol×K	883.02	Joback Method
cpg	629.65	J/mol×K	919.04	Joback Method
cpg	638.43	J/mol×K	955.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389703&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