Succinic acid, but-3-yn-2-yl 2-methoxy-5-methylphenyl ester

Inchi: InChI=1S/C16H18O5/c1-5-12(3)20-15(17)8-9-16(18)21-14-10-11(2)6-7-13(14)19-4/h1,6-

InchiKey: ZWKQJGKUYPFNDC-UHFFFAOYSA-N

Formula: C16H18O5

SMILES: C#CC(C)OC(=O)CCC(=O)Oc1cc(C)ccc1OC

Mol. weight [g/mol]: 290.31

Physical Properties

Property code	Value	Unit	Source
gf	-175.22	kJ/mol	Joback Method
hf	-495.18	kJ/mol	Joback Method
hfus	36.67	kJ/mol	Joback Method
hvap	75.00	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	2.254		Crippen Method
mcvol	224.690	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	2090.00		NIST Webbook
rinpol	2090.00		NIST Webbook
tb	766.80	K	Joback Method
tc	980.95	K	Joback Method
tf	520.06	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.93	J/mol×K	766.80	Joback Method
cpg	637.85	J/mol×K	802.49	Joback Method
cpg	650.76	J/mol×K	838.18	Joback Method
cpg	662.66	J/mol×K	873.88	Joback Method
cpg	673.55	J/mol×K	909.57	Joback Method
cpg	683.42	J/mol×K	945.26	Joback Method
cpg	692.27	J/mol×K	980.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390953&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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