Succinic acid, but-3-yn-2-yl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C15H15ClO5/c1-4-10(2)20-14(17)7-8-15(18)21-12-6-5-11(16)9-13(12)19-3/h1,

InchiKey: OEKQYXBIIGXJHW-UHFFFAOYSA-N

Formula: C15H15ClO5

SMILES: C#CC(C)OC(=O)CCC(=O)Oc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 310.73

Physical Properties

Property code	Value	Unit	Source
gf	-195.57	kJ/mol	Joback Method
hf	-490.28	kJ/mol	Joback Method
hfus	38.28	kJ/mol	Joback Method
hvap	77.16	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.599		Crippen Method
mcvol	222.840	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	2172.00		NIST Webbook
rinpol	2172.00		NIST Webbook
tb	781.35	K	Joback Method
tc	1001.31	K	Joback Method
tf	538.71	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.97	J/mol×K	781.35	Joback Method
cpg	606.39	J/mol×K	818.01	Joback Method
cpg	617.81	J/mol×K	854.67	Joback Method
cpg	628.24	J/mol×K	891.33	Joback Method
cpg	637.66	J/mol×K	927.99	Joback Method
cpg	646.09	J/mol×K	964.65	Joback Method
cpg	653.50	J/mol×K	1001.31	Joback Method

Sources

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=U390931&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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