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

Inchi: InChI=1S/C14H13ClO4/c1-3-10(2)18-13(16)7-8-14(17)19-12-6-4-5-11(15)9-12/h1,4-6,9-1

InchiKey: UDYCBZXPSXGTNI-UHFFFAOYSA-N

Formula: C14H13ClO4

SMILES: C#CC(C)OC(=O)CCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 280.70

Physical Properties

Property code	Value	Unit	Source
gf	-89.36	kJ/mol	Joback Method
hf	-325.95	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	71.86	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.590		Crippen Method
mcvol	202.880	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook
tb	731.07	K	Joback Method
tc	955.87	K	Joback Method
tf	492.69	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.09	J/mol×K	731.07	Joback Method
cpg	529.53	J/mol×K	768.54	Joback Method
cpg	541.03	J/mol×K	806.00	Joback Method
cpg	551.60	J/mol×K	843.47	Joback Method
cpg	561.28	J/mol×K	880.94	Joback Method
cpg	570.06	J/mol×K	918.40	Joback Method
cpg	577.97	J/mol×K	955.87	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=U389848&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