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

Inchi: InChI=1S/C15H15ClO4/c1-4-11(3)19-14(17)7-8-15(18)20-13-6-5-12(16)9-10(13)2/h1,5-6

InchiKey: YUYAGVZENGEQMK-UHFFFAOYSA-N

Formula: C15H15ClO4

SMILES: C#CC(C)OC(=O)CCC(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 294.73

Physical Properties

Property code	Value	Unit	Source
gf	-90.57	kJ/mol	Joback Method
hf	-358.06	kJ/mol	Joback Method
hfus	37.09	kJ/mol	Joback Method
hvap	74.75	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	2.899		Crippen Method
mcvol	216.970	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	2013.00		NIST Webbook
rinpol	2013.00		NIST Webbook
tb	758.93	K	Joback Method
tc	981.00	K	Joback Method
tf	516.48	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.37	J/mol×K	758.93	Joback Method
cpg	581.15	J/mol×K	795.94	Joback Method
cpg	592.96	J/mol×K	832.95	Joback Method
cpg	603.84	J/mol×K	869.97	Joback Method
cpg	613.78	J/mol×K	906.98	Joback Method
cpg	622.81	J/mol×K	943.99	Joback Method
cpg	630.93	J/mol×K	981.00	Joback Method

Sources

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=U390288&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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