Benzeneacetic acid, 4-chloro-, but-3-yn-2-yl ester

Inchi: InChI=1S/C12H11ClO2/c1-3-9(2)15-12(14)8-10-4-6-11(13)7-5-10/h1,4-7,9H,8H2,2H3
InchiKey: NAZJGJYUQCSYDH-UHFFFAOYSA-N
Formula: C12H11ClO2
SMILES: C#CC(C)OC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]: 222.67

Physical Properties

Property code	Value	Unit	Source
gf	127.72	kJ/mol	Joback Method
hf	-39.87	kJ/mol	Joback Method
hfus	26.92	kJ/mol	Joback Method
hvap	58.25	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.447		Crippen Method
mcvol	167.260	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
tb	609.02	K	Joback Method
tc	839.12	K	Joback Method
tf	397.99	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.92	J/mol×K	609.02	Joback Method
cpg	392.92	J/mol×K	647.37	Joback Method
cpg	405.04	J/mol×K	685.72	Joback Method
cpg	416.32	J/mol×K	724.07	Joback Method
cpg	426.79	J/mol×K	762.42	Joback Method
cpg	436.48	J/mol×K	800.77	Joback Method
cpg	445.42	J/mol×K	839.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406996&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