4-Chlorobenzoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C11H9ClO2/c1-3-8(2)14-11(13)9-4-6-10(12)7-5-9/h1,4-8H,2H3
InchiKey: LRAXWWFDHMSJAF-UHFFFAOYSA-N
Formula: C11H9ClO2
SMILES: C#CC(C)OC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 208.64

Physical Properties

Property code	Value	Unit	Source
gf	119.30	kJ/mol	Joback Method
hf	-19.23	kJ/mol	Joback Method
hfus	24.33	kJ/mol	Joback Method
hvap	56.03	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.518		Crippen Method
mcvol	153.170	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
rinpol	1419.00		NIST Webbook
tb	586.14	K	Joback Method
tc	820.90	K	Joback Method
tf	386.72	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.25	J/mol×K	586.14	Joback Method
cpg	345.40	J/mol×K	625.27	Joback Method
cpg	356.72	J/mol×K	664.39	Joback Method
cpg	367.24	J/mol×K	703.52	Joback Method
cpg	376.98	J/mol×K	742.65	Joback Method
cpg	385.98	J/mol×K	781.77	Joback Method
cpg	394.26	J/mol×K	820.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299362&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

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