2-Chlorobenzoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C12H9ClO2/c1-2-3-6-9-15-12(14)10-7-4-5-8-11(10)13/h1,3-8H,9H2
InchiKey: OYJLGUJTTGZWJG-UHFFFAOYSA-N
Formula: C12H9ClO2
SMILES: C#CC=CCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 220.65

Physical Properties

Property code	Value	Unit	Source
gf	210.38	kJ/mol	Joback Method
hf	82.63	kJ/mol	Joback Method
hfus	30.65	kJ/mol	Joback Method
hvap	58.60	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.686		Crippen Method
mcvol	162.960	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1643.00		NIST Webbook
tb	613.62	K	Joback Method
tc	848.80	K	Joback Method
tf	407.91	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.38	J/mol×K	613.62	Joback Method
cpg	370.36	J/mol×K	652.82	Joback Method
cpg	381.47	J/mol×K	692.01	Joback Method
cpg	391.76	J/mol×K	731.21	Joback Method
cpg	401.28	J/mol×K	770.41	Joback Method
cpg	410.09	J/mol×K	809.60	Joback Method
cpg	418.24	J/mol×K	848.80	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=U299299&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