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

Inchi: InChI=1S/C13H13ClO2/c1-3-7-10(4-2)16-13(15)11-8-5-6-9-12(11)14/h5-6,8-10H,4H2,1-2
InchiKey: KNDBMTMCFPSMSH-UHFFFAOYSA-N
Formula: C13H13ClO2
SMILES: CC#CC(CC)OC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 236.69

Physical Properties

Property code	Value	Unit	Source
gf	115.87	kJ/mol	Joback Method
hf	-80.11	kJ/mol	Joback Method
hfus	29.66	kJ/mol	Joback Method
hvap	62.78	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.299		Crippen Method
mcvol	181.350	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1684.00		NIST Webbook
rinpol	1684.00		NIST Webbook
tb	650.78	K	Joback Method
tc	887.00	K	Joback Method
tf	468.39	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.04	J/mol×K	650.78	Joback Method
cpg	443.25	J/mol×K	690.15	Joback Method
cpg	456.51	J/mol×K	729.52	Joback Method
cpg	468.83	J/mol×K	768.89	Joback Method
cpg	480.24	J/mol×K	808.26	Joback Method
cpg	490.77	J/mol×K	847.63	Joback Method
cpg	500.44	J/mol×K	887.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299300&Units=SI

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