Benzeneacetic acid, 4-chloro-, hex-4-yn-3-yl ester

Inchi: InChI=1S/C14H15ClO2/c1-3-5-13(4-2)17-14(16)10-11-6-8-12(15)9-7-11/h6-9,13H,4,10H

InchiKey: XFDDAQZNPQCVJV-UHFFFAOYSA-N

Formula: C14H15ClO2

SMILES: CC#CC(CC)OC(=O)Cc1ccc(Cl)cc1

Mol. weight [g/mol]: 250.72

Physical Properties

Property code	Value	Unit	Source
gf	124.29	kJ/mol	Joback Method
hf	-100.75	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	65.00	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.228		Crippen Method
mcvol	195.440	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	1801.00		NIST Webbook
rinpol	1801.00		NIST Webbook
tb	673.66	K	Joback Method
tc	905.18	K	Joback Method
tf	479.66	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.46	J/mol×K	673.66	Joback Method
cpg	494.26	J/mol×K	712.25	Joback Method
cpg	508.08	J/mol×K	750.83	Joback Method
cpg	520.93	J/mol×K	789.42	Joback Method
cpg	532.84	J/mol×K	828.00	Joback Method
cpg	543.84	J/mol×K	866.59	Joback Method
cpg	553.96	J/mol×K	905.18	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=U406998&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

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