Benzeneacetic acid, 4-chloro-, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C17H21ClO2/c1-4-5-6-16(11-13(2)3)20-17(19)12-14-7-9-15(18)10-8-14/h7-10,

InchiKey: QNOXWVIIMYSNCL-UHFFFAOYSA-N

Formula: C17H21ClO2

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

Mol. weight [g/mol]: 292.80

Physical Properties

Property code	Value	Unit	Source
gf	147.11	kJ/mol	Joback Method
hf	-167.95	kJ/mol	Joback Method
hfus	36.50	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.254		Crippen Method
mcvol	237.710	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	1975.00		NIST Webbook
rinpol	1975.00		NIST Webbook
tb	741.86	K	Joback Method
tc	965.45	K	Joback Method
tf	498.47	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	639.16	J/mol×K	741.86	Joback Method
cpg	655.49	J/mol×K	779.13	Joback Method
cpg	670.70	J/mol×K	816.39	Joback Method
cpg	684.83	J/mol×K	853.66	Joback Method
cpg	697.91	J/mol×K	890.92	Joback Method
cpg	709.99	J/mol×K	928.19	Joback Method
cpg	721.10	J/mol×K	965.45	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=U407000&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