Benzeneacetic acid, 4-chloro-, 2,7-dimethyloct-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C18H21ClO2/c1-13(2)5-10-17(11-14(3)4)21-18(20)12-15-6-8-16(19)9-7-15/h6-

InchiKey: VYHJSUIXIQWEML-UHFFFAOYSA-N

Formula: C18H21ClO2

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

Mol. weight [g/mol]: 304.81

Physical Properties

Property code	Value	Unit	Source
gf	234.82	kJ/mol	Joback Method
hf	-72.95	kJ/mol	Joback Method
hfus	36.50	kJ/mol	Joback Method
hvap	72.93	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.420		Crippen Method
mcvol	247.500	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
tb	761.30	K	Joback Method
tc	988.45	K	Joback Method
tf	494.02	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.84	J/mol×K	761.30	Joback Method
cpg	685.10	J/mol×K	799.16	Joback Method
cpg	700.22	J/mol×K	837.02	Joback Method
cpg	714.24	J/mol×K	874.88	Joback Method
cpg	727.21	J/mol×K	912.74	Joback Method
cpg	739.18	J/mol×K	950.59	Joback Method
cpg	750.19	J/mol×K	988.45	Joback Method

Sources

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=U407001&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume