2-Chlorobenzoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C17H19ClO2/c1-12(2)9-10-14(11-13(3)4)20-17(19)15-7-5-6-8-16(15)18/h5-8,1

InchiKey: KNPYXCMBMIIPQA-UHFFFAOYSA-N

Formula: C17H19ClO2

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)c1ccccc1Cl

Mol. weight [g/mol]: 290.79

Physical Properties

Property code	Value	Unit	Source
gf	226.40	kJ/mol	Joback Method
hf	-52.31	kJ/mol	Joback Method
hfus	33.91	kJ/mol	Joback Method
hvap	70.70	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.491		Crippen Method
mcvol	233.410	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	1925.00		NIST Webbook
tb	738.42	K	Joback Method
tc	969.47	K	Joback Method
tf	482.75	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.06	J/mol×K	738.42	Joback Method
cpg	630.05	J/mol×K	776.93	Joback Method
cpg	644.90	J/mol×K	815.44	Joback Method
cpg	658.67	J/mol×K	853.94	Joback Method
cpg	671.39	J/mol×K	892.45	Joback Method
cpg	683.11	J/mol×K	930.96	Joback Method
cpg	693.88	J/mol×K	969.47	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=U299303&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