2-Chlorobenzoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C16H19ClO2/c1-4-5-8-13(11-12(2)3)19-16(18)14-9-6-7-10-15(14)17/h6-7,9-10

InchiKey: OYBLJDLPLOGLEE-UHFFFAOYSA-N

Formula: C16H19ClO2

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

Mol. weight [g/mol]: 278.77

Physical Properties

Property code	Value	Unit	Source
gf	138.69	kJ/mol	Joback Method
hf	-147.31	kJ/mol	Joback Method
hfus	33.91	kJ/mol	Joback Method
hvap	69.06	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.325		Crippen Method
mcvol	223.620	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	718.98	K	Joback Method
tc	946.36	K	Joback Method
tf	487.20	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.87	J/mol×K	718.98	Joback Method
cpg	600.89	J/mol×K	756.88	Joback Method
cpg	615.80	J/mol×K	794.77	Joback Method
cpg	629.65	J/mol×K	832.67	Joback Method
cpg	642.48	J/mol×K	870.57	Joback Method
cpg	654.30	J/mol×K	908.46	Joback Method
cpg	665.17	J/mol×K	946.36	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=U299302&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume