Benzeneacetic acid, 4-chloro-, oct-3-en-2-yl ester

Inchi: InChI=1S/C16H21ClO2/c1-3-4-5-6-7-13(2)19-16(18)12-14-8-10-15(17)11-9-14/h6-11,13H

InchiKey: VCXIBZREMGTTKG-VOTSOKGWSA-N

Formula: C16H21ClO2

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

Mol. weight [g/mol]: 280.79

Physical Properties

Property code	Value	Unit	Source
gf	18.55	kJ/mol	Joback Method
hf	-297.11	kJ/mol	Joback Method
hfus	34.51	kJ/mol	Joback Method
hvap	67.26	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.561		Crippen Method
mcvol	227.920	ml/mol	McGowan Method
pc	1781.84	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	714.58	K	Joback Method
tc	924.68	K	Joback Method
tf	391.02	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.93	J/mol×K	714.58	Joback Method
cpg	622.65	J/mol×K	749.60	Joback Method
cpg	637.38	J/mol×K	784.61	Joback Method
cpg	651.17	J/mol×K	819.63	Joback Method
cpg	664.06	J/mol×K	854.64	Joback Method
cpg	676.10	J/mol×K	889.66	Joback Method
cpg	687.34	J/mol×K	924.68	Joback Method
dvisc	0.0013438	Pa×s	391.02	Joback Method

dvisc	0.0006481	Pa×s	444.95	Joback Method
dvisc	0.0003659	Pa×s	498.87	Joback Method
dvisc	0.0002310	Pa×s	552.80	Joback Method
dvisc	0.0001582	Pa×s	606.73	Joback Method
dvisc	0.0001153	Pa×s	660.65	Joback Method
dvisc	0.0000881	Pa×s	714.58	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=U406999&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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