4-Chlorobenzoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C15H19ClO2/c1-3-4-5-6-7-12(2)18-15(17)13-8-10-14(16)11-9-13/h6-12H,3-5H
InchiKey: CKYPWBNNZZHCOB-VOTSOKGWSA-N
Formula: C15H19ClO2
SMILES: CCCCC=CC(C)OC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 266.76

Physical Properties

Property code	Value	Unit	Source
gf	10.13	kJ/mol	Joback Method
hf	-276.47	kJ/mol	Joback Method
hfus	31.92	kJ/mol	Joback Method
hvap	65.03	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.632		Crippen Method
mcvol	213.830	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	1827.00		NIST Webbook
tb	691.70	K	Joback Method
tc	904.77	K	Joback Method
tf	379.75	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.39	J/mol×K	691.70	Joback Method
cpg	568.73	J/mol×K	727.21	Joback Method
cpg	583.10	J/mol×K	762.72	Joback Method
cpg	596.54	J/mol×K	798.24	Joback Method
cpg	609.10	J/mol×K	833.75	Joback Method
cpg	620.81	J/mol×K	869.26	Joback Method
cpg	631.72	J/mol×K	904.77	Joback Method
dvisc	0.0014534	Pa×s	379.75	Joback Method
dvisc	0.0007101	Pa×s	431.74	Joback Method

dvisc	0.0004047	Pa×s	483.73	Joback Method
dvisc	0.0002572	Pa×s	535.73	Joback Method
dvisc	0.0001772	Pa×s	587.72	Joback Method
dvisc	0.0001296	Pa×s	639.71	Joback Method
dvisc	0.0000994	Pa×s	691.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299366&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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