2-Chlorobenzoic acid, octyl ester

Other names: Benzoic acid, 2-chloro, octyl ester
Inchi: InChI=1S/C15H21ClO2/c1-2-3-4-5-6-9-12-18-15(17)13-10-7-8-11-14(13)16/h7-8,10-11H,
InchiKey: MBYHWDNNJFEZEI-UHFFFAOYSA-N
Formula: C15H21ClO2
SMILES: CCCCCCCCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 268.78
CAS: 97221-94-8

Physical Properties

Property code	Value	Unit	Source
gf	-67.65	kJ/mol	Joback Method
hf	-388.41	kJ/mol	Joback Method
hfus	35.24	kJ/mol	Joback Method
hvap	65.46	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.857		Crippen Method
mcvol	218.130	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1922.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1941.00		NIST Webbook
ripol	2539.00		NIST Webbook
ripol	2555.00		NIST Webbook
ripol	2566.00		NIST Webbook
ripol	2555.00		NIST Webbook
ripol	2575.00		NIST Webbook
ripol	2566.00		NIST Webbook
ripol	2532.00		NIST Webbook
ripol	2556.00		NIST Webbook
tb	687.98	K	Joback Method
tc	890.06	K	Joback Method
tf	399.83	K	Joback Method

vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.67	J/mol×K	687.98	Joback Method
cpg	644.67	J/mol×K	856.38	Joback Method
cpg	632.59	J/mol×K	822.70	Joback Method
cpg	619.68	J/mol×K	789.02	Joback Method
cpg	605.90	J/mol×K	755.34	Joback Method
cpg	591.24	J/mol×K	721.66	Joback Method
cpg	655.94	J/mol×K	890.06	Joback Method
dvisc	0.0001245	Pa×s	687.98	Joback Method
dvisc	0.0001590	Pa×s	639.96	Joback Method
dvisc	0.0002113	Pa×s	591.93	Joback Method
dvisc	0.0002954	Pa×s	543.90	Joback Method
dvisc	0.0004405	Pa×s	495.88	Joback Method
dvisc	0.0007157	Pa×s	447.86	Joback Method
dvisc	0.0013068	Pa×s	399.83	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C97221948&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume