

4-Chlorobenzoic acid, octyl ester

Other names:	Octyl 4-chlorobenzoate Benzoic acid, 4-chloro, octyl ester
Inchi:	InChI=1S/C15H21ClO2/c1-2-3-4-5-6-7-12-18-15(17)13-8-10-14(16)11-9-13/h8-11H,2-7,1
InchiKey:	JIAKTPQRGQDKAH-UHFFFAOYSA-N
Formula:	C15H21ClO2
SMILES:	CCCCCCCCOC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	268.78
CAS:	27703-70-4

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	1924.00		NIST Webbook
rinpol	1921.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1935.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1931.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1914.00		NIST Webbook
ripol	2456.00		NIST Webbook
ripol	2470.00		NIST Webbook
ripol	2466.00		NIST Webbook
ripol	2444.00		NIST Webbook
ripol	2479.00		NIST Webbook
ripol	2493.00		NIST Webbook
ripol	2470.00		NIST Webbook
tb	687.98	K	Joback Method
tc	890.06	K	Joback Method

tf	399.83	K	Joback Method
vc	0.841	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C27703704&Units=SI

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
r_{ipol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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