4-Chlorobenzoic acid, propyl ester

Other names: Propyl 4-chlorobenzoate
Benzoic acid, 4-chloro, propyl ester
Inchi: InChI=1S/C10H11ClO2/c1-2-7-13-10(12)8-3-5-9(11)6-4-8/h3-6H,2,7H2,1H3
InchiKey: BLEFFSGNRQPNCA-UHFFFAOYSA-N
Formula: C10H11ClO2
SMILES: CCCOC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 198.65
CAS: 25800-30-0

Physical Properties

Property code	Value	Unit	Source
gf	-109.75	kJ/mol	Joback Method
hf	-285.21	kJ/mol	Joback Method
hfus	22.29	kJ/mol	Joback Method
hvap	54.33	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.907		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1415.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1406.00		NIST Webbook
ripol	1948.00		NIST Webbook
ripol	1912.00		NIST Webbook
ripol	1934.00		NIST Webbook
ripol	1970.00		NIST Webbook
ripol	1974.00		NIST Webbook
ripol	1948.00		NIST Webbook
ripol	2001.00		NIST Webbook
tb	573.58	K	Joback Method
tc	791.74	K	Joback Method
tf	343.48	K	Joback Method

vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.95	J/mol×K	573.58	Joback Method
cpg	338.44	J/mol×K	609.94	Joback Method
cpg	350.20	J/mol×K	646.30	Joback Method
cpg	361.23	J/mol×K	682.66	Joback Method
cpg	371.57	J/mol×K	719.02	Joback Method
cpg	381.22	J/mol×K	755.38	Joback Method
cpg	390.20	J/mol×K	791.74	Joback Method
dvisc	0.0016661	Pa×s	343.48	Joback Method
dvisc	0.0009919	Pa×s	381.83	Joback Method
dvisc	0.0006491	Pa×s	420.18	Joback Method
dvisc	0.0004560	Pa×s	458.53	Joback Method
dvisc	0.0003383	Pa×s	496.88	Joback Method
dvisc	0.0002619	Pa×s	535.23	Joback Method
dvisc	0.0002099	Pa×s	573.58	Joback Method

Sources

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=C25800300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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