

Benzoic acid, 2-chloro, propyl ester

Inchi:	InChI=1S/C10H11ClO2/c1-2-7-13-10(12)8-5-3-4-6-9(8)11/h3-6H,2,7H2,1H3
InchiKey:	UDEIXQKSOXLXBS-UHFFFAOYSA-N
Formula:	C10H11ClO2
SMILES:	CCCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	198.65

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	1423.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1437.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1423.00		NIST Webbook
ripol	2029.00		NIST Webbook
ripol	2008.00		NIST Webbook
ripol	2046.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2058.00		NIST Webbook
ripol	2055.00		NIST Webbook
ripol	2055.00		NIST Webbook
ripol	2046.00		NIST Webbook
tb	573.58	K	Joback Method
tc	791.74	K	Joback Method
tf	343.48	K	Joback Method
vc	0.560	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R31426&Units=SI
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

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

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