Pentyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, pentyl ester
Inchi: InChI=1S/C12H15ClO2/c1-2-3-4-8-15-12(14)10-6-5-7-11(13)9-10/h5-7,9H,2-4,8H2,1H3
InchiKey: VIQQKZNPKPNBKW-UHFFFAOYSA-N
Formula: C12H15ClO2
SMILES: CCCCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 226.70

Physical Properties

Property code	Value	Unit	Source
gf	-92.91	kJ/mol	Joback Method
hf	-326.49	kJ/mol	Joback Method
hfus	27.47	kJ/mol	Joback Method
hvap	58.79	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.687		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1608.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1614.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1626.00		NIST Webbook
ripol	2166.00		NIST Webbook
ripol	2160.00		NIST Webbook
ripol	2121.00		NIST Webbook
ripol	2139.00		NIST Webbook
ripol	2153.00		NIST Webbook
ripol	2153.00		NIST Webbook
ripol	2195.00		NIST Webbook
tb	619.34	K	Joback Method
tc	830.22	K	Joback Method
tf	366.02	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.33	J/mol×K	619.34	Joback Method
cpg	483.41	J/mol×K	795.07	Joback Method
cpg	472.56	J/mol×K	759.93	Joback Method
cpg	460.94	J/mol×K	724.78	Joback Method
cpg	448.54	J/mol×K	689.63	Joback Method
cpg	435.34	J/mol×K	654.49	Joback Method
cpg	493.53	J/mol×K	830.22	Joback Method
dvisc	0.0001735	Pa×s	619.34	Joback Method
dvisc	0.0002188	Pa×s	577.12	Joback Method
dvisc	0.0002861	Pa×s	534.90	Joback Method
dvisc	0.0003918	Pa×s	492.68	Joback Method
dvisc	0.0005690	Pa×s	450.46	Joback Method
dvisc	0.0008929	Pa×s	408.24	Joback Method
dvisc	0.0015544	Pa×s	366.02	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373550&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
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