

Carbonochloridic acid, pentyl ester

Other names:	Formic acid, chloro-, pentyl ester Amyl chloroformate Chloroformic acid amyl ester Pentyl chloroformate
Inchi:	InChI=1S/C6H11ClO2/c1-2-3-4-5-9-6(7)8/h2-5H2,1H3
InchiKey:	XHRRYUDVWPPWIP-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	CCCCCOC(=O)Cl
Mol. weight [g/mol]:	150.60
CAS:	638-41-5

Physical Properties

Property code	Value	Unit	Source
gf	-246.21	kJ/mol	Joback Method
hf	-427.71	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	42.49	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.552		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpola	926.00		NIST Webbook
tb	450.40	K	Joback Method
tc	634.77	K	Joback Method
tf	259.46	K	Joback Method
vc	0.445	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.90	J/molxK	450.40	Joback Method
cpg	234.51	J/molxK	481.13	Joback Method
cpg	243.77	J/molxK	511.86	Joback Method
cpg	252.68	J/molxK	542.58	Joback Method

cpg	261.25	J/molxK	573.31	Joback Method
cpg	269.47	J/molxK	604.04	Joback Method
cpg	277.34	J/molxK	634.77	Joback Method
dvisc	0.0030315	Paxs	259.46	Joback Method
dvisc	0.0016707	Paxs	291.28	Joback Method
dvisc	0.0010354	Paxs	323.11	Joback Method
dvisc	0.0006992	Paxs	354.93	Joback Method
dvisc	0.0005036	Paxs	386.75	Joback Method
dvisc	0.0003813	Paxs	418.58	Joback Method
dvisc	0.0003003	Paxs	450.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C638415&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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