Butanoic acid, 4-chloro, pentyl ester

Other names: Pentyl 4-chlorobutanoate
Inchi: InChI=1S/C9H17ClO2/c1-2-3-4-8-12-9(11)6-5-7-10/h2-8H2,1H3
InchiKey: RCLCGTSUVBXHEE-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CCCCCOC(=O)CCCCl
Mol. weight [g/mol]: 192.68

Physical Properties

Property code	Value	Unit	Source
gf	-220.95	kJ/mol	Joback Method
hf	-489.63	kJ/mol	Joback Method
hfus	26.05	kJ/mol	Joback Method
hvap	49.17	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.739		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1301.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1317.00		NIST Webbook
tb	519.04	K	Joback Method
tc	698.13	K	Joback Method
tf	293.27	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.11	J/mol×K	519.04	Joback Method
cpg	411.03	J/mol×K	668.28	Joback Method
cpg	400.25	J/mol×K	638.43	Joback Method
cpg	388.97	J/mol×K	608.58	Joback Method

cpg	377.20	J/mol×K	578.74	Joback Method
cpg	364.91	J/mol×K	548.89	Joback Method
cpg	421.32	J/mol×K	698.13	Joback Method
dvisc	0.0002406	Pa×s	519.04	Joback Method
dvisc	0.0003106	Pa×s	481.41	Joback Method
dvisc	0.0004189	Pa×s	443.78	Joback Method
dvisc	0.0005970	Pa×s	406.15	Joback Method
dvisc	0.0009148	Pa×s	368.53	Joback Method
dvisc	0.0015445	Pa×s	330.90	Joback Method
dvisc	0.0029830	Pa×s	293.27	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R28415&Units=SI
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

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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