Butanoic acid, 4-chloro, 4-pentenyl ester

Inchi: InChI=1S/C9H15ClO2/c1-2-3-4-8-12-9(11)6-5-7-10/h2H,1,3-8H2
InchiKey: WOJRNXZZPCTQQV-UHFFFAOYSA-N
Formula: C9H15ClO2
SMILES: C=CCCCOC(=O)CCCCl
Mol. weight [g/mol]: 190.67

Physical Properties

Property code	Value	Unit	Source
gf	-133.11	kJ/mol	Joback Method
hf	-364.20	kJ/mol	Joback Method
hfus	24.77	kJ/mol	Joback Method
hvap	48.50	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.515		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	1277.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1326.00		NIST Webbook
ripol	1851.00		NIST Webbook
ripol	1865.00		NIST Webbook
ripol	1892.00		NIST Webbook
tb	515.72	K	Joback Method
tc	698.21	K	Joback Method
tf	291.51	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.64	J/mol×K	515.72	Joback Method
cpg	345.83	J/mol×K	546.14	Joback Method
cpg	357.50	J/mol×K	576.55	Joback Method

cpg	368.66	J/mol×K	606.97	Joback Method
cpg	379.31	J/mol×K	637.38	Joback Method
cpg	389.47	J/mol×K	667.80	Joback Method
cpg	399.14	J/mol×K	698.21	Joback Method
dvisc	0.0028034	Pa×s	291.51	Joback Method
dvisc	0.0014838	Pa×s	328.88	Joback Method
dvisc	0.0008942	Pa×s	366.25	Joback Method
dvisc	0.0005919	Pa×s	403.62	Joback Method
dvisc	0.0004201	Pa×s	440.98	Joback Method
dvisc	0.0003146	Pa×s	478.35	Joback Method
dvisc	0.0002457	Pa×s	515.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R28974&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume