4-Chlorobutyric acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C10H19ClO3/c1-9(5-7-13-2)8-14-10(12)4-3-6-11/h9H,3-8H2,1-2H3
InchiKey: GJHPDBDYVXVFNP-UHFFFAOYSA-N
Formula: C10H19ClO3
SMILES: COCCC(C)COC(=O)CCCCl
Mol. weight [g/mol]: 222.71

Physical Properties

Property code	Value	Unit	Source
gf	-319.97	kJ/mol	Joback Method
hf	-647.77	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	53.42	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	2.221		Crippen Method
mcvol	177.310	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1520.00		NIST Webbook
tb	563.90	K	Joback Method
tc	743.88	K	Joback Method
tf	311.77	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.53	J/mol×K	563.90	Joback Method
cpg	438.30	J/mol×K	593.90	Joback Method
cpg	451.51	J/mol×K	623.89	Joback Method
cpg	464.17	J/mol×K	653.89	Joback Method
cpg	476.27	J/mol×K	683.89	Joback Method
cpg	487.82	J/mol×K	713.89	Joback Method
cpg	498.82	J/mol×K	743.88	Joback Method
dvisc	0.0026918	Pa×s	311.77	Joback Method
dvisc	0.0012798	Pa×s	353.79	Joback Method

dvisc	0.0007126	Pa×s	395.81	Joback Method
dvisc	0.0004439	Pa×s	437.83	Joback Method
dvisc	0.0003005	Pa×s	479.86	Joback Method
dvisc	0.0002166	Pa×s	521.88	Joback Method
dvisc	0.0001639	Pa×s	563.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360641&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

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