4-Chlorooctanoic acid, methyl ester

Inchi: InChI=1S/C9H17ClO2/c1-3-4-5-8(10)6-7-9(11)12-2/h8H,3-7H2,1-2H3
InchiKey: ITHOPYACVCMDHY-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CCCCC(Cl)CCC(=O)OC
Mol. weight [g/mol]: 192.68

Physical Properties

Property code	Value	Unit	Source
gf	-223.39	kJ/mol	Joback Method
hf	-494.91	kJ/mol	Joback Method
hfus	22.53	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.737		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	1273.00		NIST Webbook
rinpol	1279.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1743.00		NIST Webbook
tb	518.60	K	Joback Method
tc	701.32	K	Joback Method
tf	278.27	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.38	J/mol×K	518.60	Joback Method
cpg	365.50	J/mol×K	549.05	Joback Method
cpg	378.08	J/mol×K	579.51	Joback Method
cpg	390.13	J/mol×K	609.96	Joback Method
cpg	401.64	J/mol×K	640.41	Joback Method
cpg	412.64	J/mol×K	670.86	Joback Method

cpg	423.11	J/mol×K	701.32	Joback Method
dvisc	0.0040831	Pa×s	278.27	Joback Method
dvisc	0.0018630	Pa×s	318.32	Joback Method
dvisc	0.0010130	Pa×s	358.38	Joback Method
dvisc	0.0006226	Pa×s	398.44	Joback Method
dvisc	0.0004182	Pa×s	438.49	Joback Method
dvisc	0.0003003	Pa×s	478.55	Joback Method
dvisc	0.0002269	Pa×s	518.60	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R309427&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume