7-Chlorononanoic acid, methyl ester

Inchi: InChI=1S/C10H19ClO2/c1-3-9(11)7-5-4-6-8-10(12)13-2/h9H,3-8H2,1-2H3
InchiKey: ROVDFFYSIOXAQH-UHFFFAOYSA-N
Formula: C10H19ClO2
SMILES: CCC(Cl)CCCCCC(=O)OC
Mol. weight [g/mol]: 206.71

Physical Properties

Property code	Value	Unit	Source
gf	-214.97	kJ/mol	Joback Method
hf	-515.55	kJ/mol	Joback Method
hfus	25.12	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.127		Crippen Method
mcvol	171.440	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1405.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	1405.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1859.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1860.00		NIST Webbook
tb	541.48	K	Joback Method
tc	722.34	K	Joback Method
tf	289.54	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.76	J/mol×K	541.48	Joback Method
cpg	412.72	J/mol×K	571.62	Joback Method

cpg	426.09	J/mol×K	601.77	Joback Method
cpg	438.88	J/mol×K	631.91	Joback Method
cpg	451.10	J/mol×K	662.05	Joback Method
cpg	462.76	J/mol×K	692.19	Joback Method
cpg	473.86	J/mol×K	722.34	Joback Method
dvisc	0.0038985	Pa×s	289.54	Joback Method
dvisc	0.0017512	Pa×s	331.53	Joback Method
dvisc	0.0009417	Pa×s	373.52	Joback Method
dvisc	0.0005741	Pa×s	415.51	Joback Method
dvisc	0.0003832	Pa×s	457.50	Joback Method
dvisc	0.0002738	Pa×s	499.49	Joback Method
dvisc	0.0002061	Pa×s	541.48	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R309769&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