CHLOROMETHYL 3-CHLORO-OCTANOATE

Other names: 3-Chlorooctanoic acid, chloromethyl ester
Inchi: InChI=1S/C9H16Cl2O2/c1-2-3-4-5-8(11)6-9(12)13-7-10/h8H,2-7H2,1H3
InchiKey: QVLVXAKSGCMENB-UHFFFAOYSA-N
Formula: C9H16Cl2O2
SMILES: CCCCCC(Cl)CC(=O)OCCl
Mol. weight [g/mol]: 227.13

Physical Properties

Property code	Value	Unit	Source
hf	-598.77	kJ/mol	Cheméo Relay (1.0)
hfus	26.72	kJ/mol	Joback Method
hvap	64.44	kJ/mol	Cheméo Relay (1.0)
logp	3.304		Crippen Method
mcvol	169.590	ml/mol	McGowan Method
rinpol	1425.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1425.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	1969.00		NIST Webbook
tb	514.04	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.33	J/mol×K	556.03	Joback Method
cpg	392.87	J/mol×K	587.29	Joback Method
cpg	404.84	J/mol×K	618.56	Joback Method
cpg	416.25	J/mol×K	649.82	Joback Method
cpg	427.10	J/mol×K	681.08	Joback Method
cpg	437.41	J/mol×K	712.35	Joback Method
cpg	447.18	J/mol×K	743.61	Joback Method

dvisc	0.0034137	Pa×s	308.19	Joback Method
dvisc	0.0016431	Pa×s	349.50	Joback Method
dvisc	0.0009231	Pa×s	390.80	Joback Method
dvisc	0.0005790	Pa×s	432.11	Joback Method
dvisc	0.0003940	Pa×s	473.42	Joback Method
dvisc	0.0002852	Pa×s	514.72	Joback Method
dvisc	0.0002166	Pa×s	556.03	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418651&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature