CHLOROMETHYL NONANOATE

Other names: Nonanoic acid, chloromethyl ester
Inchi: InChI=1S/C10H19ClO2/c1-2-3-4-5-6-7-8-10(12)13-9-11/h2-9H2,1H3
InchiKey: NNVIRQBZFULPEI-UHFFFAOYSA-N
Formula: C10H19ClO2
SMILES: CCCCCCCCC(=O)OCCl
Mol. weight [g/mol]: 206.71

Physical Properties

Property code	Value	Unit	Source
af	0.6527		Cheméo Relay (1.0)
hf	-604.95	kJ/mol	Cheméo Relay (1.0)
hfus	28.64	kJ/mol	Joback Method
hvap	63.35	kJ/mol	Cheméo Relay (1.0)
ie	9.90	eV	Cheméo Relay (1.0)
log10ws	-4.17		Cheméo Relay (1.0)
logp	3.476		Crippen Method
mcvol	171.440	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	1380.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1364.00		NIST Webbook
ripol	1796.00		NIST Webbook
ripol	1776.00		NIST Webbook
ripol	1798.00		NIST Webbook
ripol	1776.00		NIST Webbook
tb	513.36	K	Cheméo Relay (1.0)
tc	698.06	K	Cheméo Relay (1.0)
tf	247.66	K	Cheméo Relay (1.0)
vc	0.648	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.46	J/mol×K	541.92	Joback Method

cpg	412.10	J/mol×K	571.49	Joback Method
cpg	425.18	J/mol×K	601.06	Joback Method
cpg	437.70	J/mol×K	630.63	Joback Method
cpg	449.68	J/mol×K	660.20	Joback Method
cpg	461.13	J/mol×K	689.77	Joback Method
cpg	472.05	J/mol×K	719.34	Joback Method
dvisc	0.0028840	Pa×s	304.54	Joback Method
dvisc	0.0014664	Pa×s	344.10	Joback Method
dvisc	0.0008572	Pa×s	383.67	Joback Method
dvisc	0.0005540	Pa×s	423.23	Joback Method
dvisc	0.0003858	Pa×s	462.79	Joback Method
dvisc	0.0002844	Pa×s	502.36	Joback Method
dvisc	0.0002192	Pa×s	541.92	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77877953&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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