

Chloromethyl 9-chlorononanoate

Other names:	9-Chlorononanoic acid, chloromethyl ester
Inchi:	InChI=1S/C10H18Cl2O2/c11-8-6-4-2-1-3-5-7-10(13)14-9-12/h1-9H2
InchiKey:	AAVUFTKCHHFPHZ-UHFFFAOYSA-N
Formula:	C10H18Cl2O2
SMILES:	O=C(CCCCCCCCCI)OCCI
Mol. weight [g/mol]:	241.16
CAS:	80418-78-6

Physical Properties

Property code	Value	Unit	Source
gf	-224.46	kJ/mol	Joback Method
hf	-526.01	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	55.78	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.695		Crippen Method
mcvol	183.680	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1657.00		NIST Webbook
ripol	2255.00		NIST Webbook
ripol	2286.00		NIST Webbook
ripol	2302.00		NIST Webbook
tb	579.35	K	Joback Method
tc	761.47	K	Joback Method
tf	334.46	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.35	J/molxK	579.35	Joback Method
cpg	440.37	J/molxK	609.70	Joback Method

cpg	452.81	J/molxK	640.06	Joback Method
cpg	464.67	J/molxK	670.41	Joback Method
cpg	475.97	J/molxK	700.77	Joback Method
cpg	486.72	J/molxK	731.12	Joback Method
cpg	496.91	J/molxK	761.47	Joback Method
dvisc	0.0024726	Paxs	334.46	Joback Method
dvisc	0.0013060	Paxs	375.28	Joback Method
dvisc	0.0007818	Paxs	416.09	Joback Method
dvisc	0.0005129	Paxs	456.90	Joback Method
dvisc	0.0003606	Paxs	497.72	Joback Method
dvisc	0.0002675	Paxs	538.53	Joback Method
dvisc	0.0002069	Paxs	579.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418786&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

Latest version available from:

<https://www.chemeo.com/cid/68-121-2/Chloromethyl-9-chlorononanoate.pdf>

Generated by Cheméo on 2024-05-09 08:12:32.16936792 +0000 UTC m=+17531601.089945242.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.