Nonanoyl chloride

Other names:	Pelargonoyl chloride
	Nonanoic acid chloride
Inchi:	InChI=1S/C9H17ClO/c1-2-3-4-5-6-7-8-9(10)11/h2-8H2,1H3
InchiKey:	NTQYXUJLILNTFH-UHFFFAOYSA-N
Formula:	C9H17ClO
SMILES:	CCCCCCCCC(=O)Cl
Mol. weight [g/mol]:	176.68
CAS:	764-85-2

Physical Properties

Property code	Value	Unit	Source
gf	-115.95	kJ/mol	Joback Method
hf	-357.41	kJ/mol	Joback Method
hfus	24.86	kJ/mol	Joback Method
hvap	46.76	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.502		Crippen Method
mcvol	151.480	ml/mol	McGowan Method
pc	2365.67	kPa	Joback Method
rinpol	1215.70		NIST Webbook
tb	493.15 ± 6.00	K	NIST Webbook
tb	487.00 ± 10.00	K	NIST Webbook
tb	488.50	K	NIST Webbook
tc	676.51	K	Joback Method
tf	271.04	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.38	J/mol×K	496.62	Joback Method
cpg	340.41	J/mol×K	526.60	Joback Method
cpg	352.87	J/mol×K	556.58	Joback Method
cpg	364.77	J/mol×K	586.56	Joback Method

cpg	376.14	J/mol×K	616.55	Joback Method
cpg	386.99	J/mol×K	646.53	Joback Method
cpg	397.34	J/mol×K	676.51	Joback Method
dvisc	0.0041228	Pa×s	271.04	Joback Method
dvisc	0.0020309	Pa×s	308.64	Joback Method
dvisc	0.0011667	Pa×s	346.23	Joback Method
dvisc	0.0007472	Pa×s	383.83	Joback Method
dvisc	0.0005181	Pa×s	421.43	Joback Method
dvisc	0.0003814	Pa×s	459.02	Joback Method
dvisc	0.0002942	Pa×s	496.62	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.20	K	2.90	NIST Webbook
tbrp	371.20	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C764852&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume