Azelaoyl chloride

Other names:	Nonanedioyl dichloride
	Azelaic acid chloride
	Azelayl chloride
	Azeoloyl chloride
Inchi:	InChI=1S/C9H14Cl2O2/c10-8(12)6-4-2-1-3-5-7-9(11)13/h1-7H2
InchiKey:	HGEVGSTXQGZPCL-UHFFFAOYSA-N
Formula:	C9H14Cl2O2
SMILES:	O=C(Cl)CCCCCCCC(=O)Cl
Mol. weight [g/mol]:	225.11
CAS:	123-98-8

Physical Properties

Property code	Value	Unit	Source
gf	-256.80	kJ/mol	Joback Method
hf	-485.73	kJ/mol	Joback Method
hfus	30.66	kJ/mol	Joback Method
hvap	57.89	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.248		Crippen Method
mcvol	165.290	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
tb	587.92	K	Joback Method
tc	781.09	K	Joback Method
tf	350.89	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.48	J/mol×K	587.92	Joback Method
cpg	383.89	J/mol×K	620.11	Joback Method
cpg	394.70	J/mol×K	652.31	Joback Method
cpg	404.93	J/mol×K	684.50	Joback Method
cpg	414.59	J/mol×K	716.70	Joback Method

cpg	423.70	J/mol×K	748.89	Joback Method
cpg	432.29	J/mol×K	781.09	Joback Method
dvisc	0.0029474	Pa×s	350.89	Joback Method
dvisc	0.0016590	Pa×s	390.39	Joback Method
dvisc	0.0010378	Pa×s	429.90	Joback Method
dvisc	0.0007025	Pa×s	469.40	Joback Method
dvisc	0.0005053	Pa×s	508.91	Joback Method
dvisc	0.0003811	Pa×s	548.41	Joback Method
dvisc	0.0002985	Pa×s	587.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	439.20	K	2.40	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C123988&Units=SI

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

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume