Pimeloyl chloride

Other names: Heptanedioyl dichloride
Inchi: InChI=1S/C7H10Cl2O2/c8-6(10)4-2-1-3-5-7(9)11/h1-5H2
InchiKey: LVIMBOHJGMDKEJ-UHFFFAOYSA-N
Formula: C7H10Cl2O2
SMILES: O=C(Cl)CCCCCC(=O)Cl
Mol. weight [g/mol]: 197.06

Physical Properties

Property code	Value	Unit	Source
hf	-490.53	kJ/mol	Cheméo Relay (1.0)
hfus	25.48	kJ/mol	Joback Method
hvap	60.36	kJ/mol	Cheméo Relay (1.0)
ie	10.04	eV	Cheméo Relay (1.0)
log10ws	-3.14		Cheméo Relay (1.0)
logp	2.468		Crippen Method
mcvol	137.110	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	498.21	K	Cheméo Relay (1.0)
tf	298.13	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.18	J/mol×K	542.16	Joback Method
cpg	291.80	J/mol×K	575.22	Joback Method
cpg	300.91	J/mol×K	608.28	Joback Method
cpg	309.52	J/mol×K	641.34	Joback Method
cpg	317.65	J/mol×K	674.41	Joback Method
cpg	325.30	J/mol×K	707.47	Joback Method
cpg	332.50	J/mol×K	740.53	Joback Method
dvisc	0.0031969	Pa×s	328.35	Joback Method
dvisc	0.0018666	Pa×s	363.99	Joback Method
dvisc	0.0011996	Pa×s	399.62	Joback Method
dvisc	0.0008289	Pa×s	435.25	Joback Method

dvisc	0.0006056	Pa×s	470.89	Joback Method
dvisc	0.0004625	Pa×s	506.52	Joback Method
dvisc	0.0003660	Pa×s	542.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.20	K	0.70	NIST Webbook
tbrp	410.20	K	2.00	NIST Webbook

Sources

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=C142790&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
ie: Ionization energy
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
tf: Normal melting (fusion) point