

Pimeloylchloride

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)CCCCC(=O)Cl
Mol. weight [g/mol]:	197.06
CAS:	142-79-0

Physical Properties

Property code	Value	Unit	Source
gf	-273.64	kJ/mol	Joback Method
hf	-444.45	kJ/mol	Joback Method
hfus	25.48	kJ/mol	Joback Method
hvap	53.44	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.468		Crippen Method
mcvol	137.110	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	542.16	K	Joback Method
tc	740.53	K	Joback Method
tf	328.35	K	Joback Method
vc	0.537	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C142790&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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