Hexanedioyl dichloride

Other names:	Adipoyl chloride
	Adipic acid dichloride
	Adipic dichloride
	Adipoyl dichloride
	Adipyl chloride
	Hexanedioyl chloride
	1,4-Bis(Chlorocarbonyl)butane
Inchi:	InChI=1S/C6H8Cl2O2/c7-5(9)3-1-2-4-6(8)10/h1-4H2
InchiKey:	PWAXUOGZOSVGBO-UHFFFAOYSA-N
Formula:	C6H8Cl2O2
SMILES:	O=C(Cl)CCCCC(=O)Cl
Mol. weight [g/mol]:	183.03
CAS:	111-50-2

Physical Properties

Property code	Value	Unit	Source
gf	-282.06	kJ/mol	Joback Method
hf	-423.81	kJ/mol	Joback Method
hfus	22.89	kJ/mol	Joback Method
hvap	51.21	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.078		Crippen Method
mcvol	123.020	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	519.28	K	Joback Method
tc	720.45	K	Joback Method
tf	317.08	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.78	J/mol×K	519.28	Joback Method
cpg	248.34	J/mol×K	552.81	Joback Method

cpg	256.43	J/mol×K	586.34	Joback Method
cpg	264.07	J/mol×K	619.87	Joback Method
cpg	271.28	J/mol×K	653.40	Joback Method
cpg	278.06	J/mol×K	686.92	Joback Method
cpg	284.43	J/mol×K	720.45	Joback Method
dvisc	0.0032730	Pa×s	317.08	Joback Method
dvisc	0.0019493	Pa×s	350.78	Joback Method
dvisc	0.0012714	Pa×s	384.48	Joback Method
dvisc	0.0008883	Pa×s	418.18	Joback Method
dvisc	0.0006548	Pa×s	451.88	Joback Method
dvisc	0.0005035	Pa×s	485.58	Joback Method
dvisc	0.0004006	Pa×s	519.28	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.20	K	0.30	NIST Webbook

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=C111502&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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