

6-Chloropiperonyl chloride

Other names:	1,3-Benzodioxole, 5-chloro-6-(chloromethyl)-
Inchi:	InChI=1S/C8H6Cl2O2/c9-3-5-1-7-8(2-6(5)10)12-4-11-7/h1-2H,3-4H2
InchiKey:	APJKOQPCHGXQBI-UHFFFAOYSA-N
Formula:	C8H6Cl2O2
SMILES:	ClCc1cc2c(cc1Cl)OCO2
Mol. weight [g/mol]:	205.04
CAS:	23468-31-7

Physical Properties

Property code	Value	Unit	Source
gf	-27.64	kJ/mol	Joback Method
hf	-208.67	kJ/mol	Joback Method
hfus	30.77	kJ/mol	Joback Method
hvap	55.68	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.808		Crippen Method
mcvol	125.180	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
tb	564.23	K	Joback Method
tc	804.19	K	Joback Method
tf	379.06	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.47	J/molxK	564.23	Joback Method
cpg	269.02	J/molxK	604.22	Joback Method
cpg	277.82	J/molxK	644.22	Joback Method
cpg	285.94	J/molxK	684.21	Joback Method
cpg	293.43	J/molxK	724.20	Joback Method
cpg	300.35	J/molxK	764.20	Joback Method
cpg	306.78	J/molxK	804.19	Joback Method
dvisc	0.0018667	Paxs	379.06	Joback Method

dvisc	0.0013936	Paxs	409.92	Joback Method
dvisc	0.0010839	Paxs	440.78	Joback Method
dvisc	0.0008712	Paxs	471.64	Joback Method
dvisc	0.0007193	Paxs	502.51	Joback Method
dvisc	0.0006071	Paxs	533.37	Joback Method
dvisc	0.0005221	Paxs	564.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C23468317&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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