

6-Chloropiperonal

Other names:	6-Chloro-3,4-methylene dioxy benzaldehyde
Inchi:	InChI=1S/C8H5ClO3/c9-6-2-8-7(11-4-12-8)1-5(6)3-10/h1-3H,4H2
InchiKey:	VRNADRCOROWLJC-UHFFFAOYSA-N
Formula:	C8H5ClO3
SMILES:	O=Cc1cc2c(cc1Cl)OCO2
Mol. weight [g/mol]:	184.58
CAS:	15952-61-1

Physical Properties

Property code	Value	Unit	Source
gf	-115.23	kJ/mol	Joback Method
hf	-278.51	kJ/mol	Joback Method
hfus	28.86	kJ/mol	Joback Method
hvap	58.01	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.881		Crippen Method
mcvol	114.510	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	575.46	K	Joback Method
tc	813.59	K	Joback Method
tf	391.14	K	Joback Method
vc	0.442	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.11	J/molxK	575.46	Joback Method
cpg	257.92	J/molxK	615.15	Joback Method
cpg	266.03	J/molxK	654.84	Joback Method
cpg	273.50	J/molxK	694.52	Joback Method
cpg	280.38	J/molxK	734.21	Joback Method
cpg	286.73	J/molxK	773.90	Joback Method
cpg	292.61	J/molxK	813.59	Joback Method
dvisc	0.0021247	Paxs	391.14	Joback Method

dvisc	0.0016091	Paxs	421.86	Joback Method
dvisc	0.0012655	Paxs	452.58	Joback Method
dvisc	0.0010261	Paxs	483.30	Joback Method
dvisc	0.0008532	Paxs	514.02	Joback Method
dvisc	0.0007243	Paxs	544.74	Joback Method
dvisc	0.0006257	Paxs	575.46	Joback Method

Sources

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=C15952611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	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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