

2-Chloroisovaleric acid

Inchi:	InChI=1S/C5H9ClO2/c1-3(2)4(6)5(7)8/h3-4H,1-2H3,(H,7,8)
InchiKey:	DDTJFSPKEIAZAM-UHFFFAOYSA-N
Formula:	C5H9ClO2
SMILES:	CC(C)C(Cl)C(=O)O
Mol. weight [g/mol]:	136.58
CAS:	921-08-4

Physical Properties

Property code	Value	Unit	Source
gf	-291.33	kJ/mol	Joback Method
hf	-437.64	kJ/mol	Joback Method
hfus	11.54	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	1.334		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	4088.15	kPa	Joback Method
tb	496.40	K	Joback Method
tc	682.37	K	Joback Method
tf	256.78	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.76	J/molxK	496.40	Joback Method
cpg	242.57	J/molxK	651.37	Joback Method
cpg	236.13	J/molxK	620.38	Joback Method
cpg	229.33	J/molxK	589.38	Joback Method
cpg	222.18	J/molxK	558.39	Joback Method
cpg	214.66	J/molxK	527.39	Joback Method
cpg	248.69	J/molxK	682.37	Joback Method
dvisc	0.0001957	Paxs	496.40	Joback Method
dvisc	0.0003318	Paxs	456.46	Joback Method

dvisc	0.0006223	Paxs	416.53	Joback Method
dvisc	0.0013336	Paxs	376.59	Joback Method
dvisc	0.0034247	Paxs	336.65	Joback Method
dvisc	0.0113364	Paxs	296.72	Joback Method
dvisc	0.0544542	Paxs	256.78	Joback Method

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=C921084&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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