

Butanoyl chloride, 3-methyl-

Other names:	Isovaleryl chloride Isopentanoyl chloride Isovaleric acid chloride Isovaleric chloride Isovaleroyl chloride 3-Methylbutanoyl chloride 3-Methylbutyryl chloride
Inchi:	InChI=1S/C5H9ClO/c1-4(2)3-5(6)7/h4H,3H2,1-2H3
InchiKey:	ISULZYQDGYXDFW-UHFFFAOYSA-N
Formula:	C5H9ClO
SMILES:	CC(C)CC(=O)Cl
Mol. weight [g/mol]:	120.58
CAS:	108-12-3

Physical Properties

Property code	Value	Unit	Source
gf	-152.07	kJ/mol	Joback Method
hf	-280.13	kJ/mol	Joback Method
hfus	10.98	kJ/mol	Joback Method
hvap	37.47	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.798		Crippen Method
mvol	95.120	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	757.60		NIST Webbook
tb	389.20	K	NIST Webbook
tc	595.49	K	Joback Method
tf	210.96	K	Joback Method
vc	0.364	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.21	J/mol×K	404.66	Joback Method

cpg	206.34	J/molxK	563.69	Joback Method
cpg	199.04	J/molxK	531.88	Joback Method
cpg	191.40	J/molxK	500.08	Joback Method
cpg	183.38	J/molxK	468.27	Joback Method
cpg	174.99	J/molxK	436.47	Joback Method
cpg	213.28	J/molxK	595.49	Joback Method
dvisc	0.0003464	Paxs	404.66	Joback Method
dvisc	0.0004515	Paxs	372.38	Joback Method
dvisc	0.0006188	Paxs	340.09	Joback Method
dvisc	0.0009061	Paxs	307.81	Joback Method
dvisc	0.0014508	Paxs	275.53	Joback Method
dvisc	0.0026320	Paxs	243.24	Joback Method
dvisc	0.0057299	Paxs	210.96	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=C108123&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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