isobutyryl chloride

Other names: 2-Methylpropanoyl chloride
Inchi: InChI=1S/C4H7ClO/c1-3(2)4(5)6/h3H,1-2H3
InchiKey: DGMOBVGABMBZSB-UHFFFAOYSA-N
Formula: C4H7ClO
SMILES: CC(C)C(=O)Cl
Mol. weight [g/mol]: 106.55
CAS: 79-30-1

Physical Properties

Property code	Value	Unit	Source
gf	-160.49	kJ/mol	Joback Method
hf	-259.49	kJ/mol	Joback Method
hfus	8.39	kJ/mol	Joback Method
hvap	35.24	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	1.408		Crippen Method
mcvol	81.030	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpol	672.00		NIST Webbook
rinpol	672.00		NIST Webbook
rinpol	672.00		NIST Webbook
tb	365.00 ± 2.00	K	NIST Webbook
tb	333.00 ± 4.00	K	NIST Webbook
tb	363.00 ± 3.00	K	NIST Webbook
tb	365.20	K	NIST Webbook
tc	573.96	K	Joback Method
tf	183.20 ± 0.70	K	NIST Webbook
vc	0.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.55	J/mol×K	381.78	Joback Method
cpg	138.84	J/mol×K	413.81	Joback Method

cpg	145.81	J/mol×K	445.84	Joback Method
cpg	152.47	J/mol×K	477.87	Joback Method
cpg	158.83	J/mol×K	509.90	Joback Method
cpg	164.89	J/mol×K	541.93	Joback Method
cpg	170.67	J/mol×K	573.96	Joback Method
cpl	131.80	J/mol×K	298.00	NIST Webbook
dvisc	0.0053672	Pa×s	199.69	Joback Method
dvisc	0.0025233	Pa×s	230.04	Joback Method
dvisc	0.0014145	Pa×s	260.39	Joback Method
dvisc	0.0008947	Pa×s	290.74	Joback Method
dvisc	0.0006172	Pa×s	321.08	Joback Method
dvisc	0.0004539	Pa×s	351.43	Joback Method
dvisc	0.0003505	Pa×s	381.78	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C79301&Units=SI

Legend

cpg: Ideal gas heat capacity

cpl: Liquid phase 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