2,2-Dimethylvaleroyl chloride

Other names: Pentanoyl chloride, 2,2-dimethyl-
Inchi: InChI=1S/C7H13ClO/c1-4-5-7(2,3)6(8)9/h4-5H2,1-3H3
InchiKey: NUBKYCCXDNYHLQ-UHFFFAOYSA-N
Formula: C7H13ClO
SMILES: CCCC(C)(C)C(=O)Cl
Mol. weight [g/mol]: 148.63
CAS: 15721-22-9

Physical Properties

Property code	Value	Unit	Source
gf	-129.95	kJ/mol	Joback Method
hf	-324.88	kJ/mol	Joback Method
hfus	12.27	kJ/mol	Joback Method
hvap	41.01	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.578		Crippen Method
mcvol	123.300	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
tb	447.63	K	Joback Method
tc	642.91	K	Joback Method
tf	250.92	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.14	J/mol×K	447.63	Joback Method
cpg	257.32	J/mol×K	480.18	Joback Method
cpg	268.82	J/mol×K	512.72	Joback Method
cpg	279.66	J/mol×K	545.27	Joback Method
cpg	289.87	J/mol×K	577.82	Joback Method
cpg	299.49	J/mol×K	610.36	Joback Method
cpg	308.55	J/mol×K	642.91	Joback Method
dvisc	0.0059406	Pa×s	250.92	Joback Method

dvisc	0.0028073	Pa×s	283.71	Joback Method
dvisc	0.0015495	Pa×s	316.49	Joback Method
dvisc	0.0009562	Pa×s	349.27	Joback Method
dvisc	0.0006410	Pa×s	382.06	Joback Method
dvisc	0.0004578	Pa×s	414.85	Joback Method
dvisc	0.0003435	Pa×s	447.63	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.50 ± 0.50	K	4.00	NIST Webbook

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=C15721229&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume