

2-Methylvaleryl chloride

Other names:	2-Methylvaleroyl chloride
Inchi:	InChI=1S/C6H11ClO/c1-3-4-5(2)6(7)8/h5H,3-4H2,1-2H3
InchiKey:	MFIQXAVMTLKUJR-UHFFFAOYSA-N
Formula:	C6H11ClO
SMILES:	CCCC(C)C(=O)Cl
Mol. weight [g/mol]:	134.61

Physical Properties

Property code	Value	Unit	Source
hf	-324.94	kJ/mol	Cheméo Relay (1.0)
hfus	13.57	kJ/mol	Joback Method
hvap	38.45	kJ/mol	Cheméo Relay (1.0)
ie	9.97	eV	Cheméo Relay (1.0)
log10ws	-2.31		Cheméo Relay (1.0)
logp	2.188		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
tb	413.50 ± 1.50	K	NIST Webbook
tc	583.97	K	Cheméo Relay (1.0)
tf	176.11	K	Cheméo Relay (1.0)
vc	0.389	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.25	J/mol×K	427.54	Joback Method
cpg	213.38	J/mol×K	459.08	Joback Method
cpg	223.06	J/mol×K	490.62	Joback Method
cpg	232.30	J/mol×K	522.16	Joback Method
cpg	241.12	J/mol×K	553.70	Joback Method
cpg	249.52	J/mol×K	585.24	Joback Method
cpg	257.52	J/mol×K	616.78	Joback Method
dvisc	0.0059488	Pa×s	222.23	Joback Method
dvisc	0.0026756	Pa×s	256.45	Joback Method

dvisc	0.0014525	Pa×s	290.67	Joback Method
dvisc	0.0008968	Pa×s	324.88	Joback Method
dvisc	0.0006070	Pa×s	359.10	Joback Method
dvisc	0.0004397	Pa×s	393.32	Joback Method
dvisc	0.0003354	Pa×s	427.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5238277&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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