

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]:	134.60
CAS:	5238-27-7

Physical Properties

Property code	Value	Unit	Source
gf	-143.65	kJ/mol	Joback Method
hf	-300.77	kJ/mol	Joback Method
hfus	13.57	kJ/mol	Joback Method
hvap	39.69	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
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	616.78	K	Joback Method
tf	222.23	K	Joback Method
vc	0.420	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.25	J/mol×K	427.54	Joback Method
cpg	249.52	J/mol×K	585.24	Joback Method
cpg	241.12	J/mol×K	553.70	Joback Method
cpg	232.30	J/mol×K	522.16	Joback Method
cpg	223.06	J/mol×K	490.62	Joback Method
cpg	213.38	J/mol×K	459.08	Joback Method
cpg	257.52	J/mol×K	616.78	Joback Method
dvisc	0.0003354	Paxs	427.54	Joback Method

dvisc	0.0004397	Paxs	393.32	Joback Method
dvisc	0.0006070	Paxs	359.10	Joback Method
dvisc	0.0008968	Paxs	324.88	Joback Method
dvisc	0.0014525	Paxs	290.67	Joback Method
dvisc	0.0026756	Paxs	256.45	Joback Method
dvisc	0.0059488	Paxs	222.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5238277&Units=SI
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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/80-999-5/2-methylvaleryl-chloride.pdf>

Generated by Cheméo on 2024-04-20 05:08:19.002077796 +0000 UTC m=+15878947.922655117.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.