

Methyl 4-chloropentanoate

Other names:	Methyl 4-chloropentanoate
Inchi:	InChI=1S/C6H11ClO2/c1-5(7)3-4-6(8)9-2/h5H,3-4H2,1-2H3
InchiKey:	UHNCLQCIKXIBSA-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	COC(=O)CCC(C)Cl
Mol. weight [g/mol]:	150.61

Physical Properties

Property code	Value	Unit	Source
af	0.4377		Cheméo Relay (1.0)
hf	-509.17	kJ/mol	Cheméo Relay (1.0)
hfus	14.76	kJ/mol	Joback Method
hvap	53.10	kJ/mol	Cheméo Relay (1.0)
ie	10.19	eV	Cheméo Relay (1.0)
log10ws	-1.30		Cheméo Relay (1.0)
logp	1.567		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	983.00		NIST Webbook
rinpol	983.00		NIST Webbook
ripol	1475.00		NIST Webbook
ripol	1431.00		NIST Webbook
ripol	1431.00		NIST Webbook
tb	439.65	K	Cheméo Relay (1.0)
tc	623.06	K	Cheméo Relay (1.0)
tf	215.80	K	Cheméo Relay (1.0)
vc	0.413	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.04	J/mol×K	449.96	Joback Method
cpg	234.96	J/mol×K	481.38	Joback Method
cpg	244.50	J/mol×K	512.81	Joback Method

cpg	253.66	J/mol×K	544.23	Joback Method
cpg	262.46	J/mol×K	575.65	Joback Method
cpg	270.88	J/mol×K	607.08	Joback Method
cpg	278.93	J/mol×K	638.50	Joback Method
dvisc	0.0043249	Pa×s	244.46	Joback Method
dvisc	0.0020836	Pa×s	278.71	Joback Method
dvisc	0.0011778	Pa×s	312.96	Joback Method
dvisc	0.0007450	Pa×s	347.21	Joback Method
dvisc	0.0005117	Pa×s	381.46	Joback Method
dvisc	0.0003739	Pa×s	415.71	Joback Method
dvisc	0.0002866	Pa×s	449.96	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63318207&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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