3-Methylbutyl 4-chlorobutyrate

Other names: 3-Methylbutyl 4-chlorobutyrate
Inchi: InChI=1S/C9H17ClO2/c1-8(2)5-7-12-9(11)4-3-6-10/h8H,3-7H2,1-2H3
InchiKey: AIQWYBIIHIAUKD-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CC(C)CCOC(=O)CCCCl
Mol. weight [g/mol]: 192.69

Physical Properties

Property code	Value	Unit	Source
chl	-5338.40 ± 8.40	kJ/mol	NIST Webbook
chl	-5327.90	kJ/mol	NIST Webbook
hf	-600.80 ± 9.60	kJ/mol	NIST Webbook
hfl	-656.50 ± 8.40	kJ/mol	NIST Webbook
hfus	22.53	kJ/mol	Joback Method
hvap	55.60 ± 4.20	kJ/mol	NIST Webbook
ie	10.05	eV	Cheméo Relay (1.0)
log10ws	-2.75		Cheméo Relay (1.0)
logp	2.595		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	1306.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1274.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1706.00		NIST Webbook
tb	489.45	K	Cheméo Relay (1.0)
tc	677.11	K	Cheméo Relay (1.0)
tf	206.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.38	J/mol×K	518.60	Joback Method
cpg	365.50	J/mol×K	549.05	Joback Method
cpg	378.08	J/mol×K	579.51	Joback Method
cpg	390.13	J/mol×K	609.96	Joback Method
cpg	401.64	J/mol×K	640.41	Joback Method
cpg	412.64	J/mol×K	670.86	Joback Method
cpg	423.11	J/mol×K	701.32	Joback Method
dvisc	0.0040831	Pa×s	278.27	Joback Method
dvisc	0.0018630	Pa×s	318.32	Joback Method
dvisc	0.0010130	Pa×s	358.38	Joback Method
dvisc	0.0006226	Pa×s	398.43	Joback Method
dvisc	0.0004182	Pa×s	438.49	Joback Method
dvisc	0.0003003	Pa×s	478.54	Joback Method
dvisc	0.0002269	Pa×s	518.60	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62108809&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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