

Butanoic acid, 4-chloro, 3-methylbutyl ester

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]:	192.68
CAS:	62108-80-9

Physical Properties

Property code	Value	Unit	Source
chl	-5327.90	kJ/mol	NIST Webbook
chl	-5338.40 ± 8.40	kJ/mol	NIST Webbook
gf	-223.39	kJ/mol	Joback Method
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
log10ws	-2.36		Crippen Method
logp	2.595		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	1256.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1306.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1690.00		NIST Webbook
tb	518.60	K	Joback Method
tc	701.32	K	Joback Method
tf	278.27	K	Joback Method
vc	0.607	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.38	J/molxK	518.60	Joback Method
cpg	365.50	J/molxK	549.05	Joback Method
cpg	378.08	J/molxK	579.51	Joback Method
cpg	390.13	J/molxK	609.96	Joback Method
cpg	401.64	J/molxK	640.41	Joback Method
cpg	412.64	J/molxK	670.86	Joback Method
cpg	423.11	J/molxK	701.32	Joback Method
dvisc	0.0040831	Paxs	278.27	Joback Method
dvisc	0.0018630	Paxs	318.32	Joback Method
dvisc	0.0010130	Paxs	358.38	Joback Method
dvisc	0.0006226	Paxs	398.44	Joback Method
dvisc	0.0004182	Paxs	438.49	Joback Method
dvisc	0.0003003	Paxs	478.55	Joback Method
dvisc	0.0002269	Paxs	518.60	Joback Method

Sources

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=C62108809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
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
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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