

Acetic acid, chloro-, butyl ester

Other names:	n-Butyl chloroacetate Butyl chloroacetate Chloroacetic acid butyl ester Monochloroacetic acid n-butyl ester Chloroacetic acid n-butyl ester 2-Chloroacetic acid, n-butyl ester
Inchi:	InChI=1S/C6H11ClO2/c1-2-3-4-9-6(8)5-7/h2-5H2,1H3
InchiKey:	YJRGMUWRPCPLNH-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	CCCCOC(=O)CCl
Mol. weight [g/mol]:	150.60
CAS:	590-02-3

Physical Properties

Property code	Value	Unit	Source
chl	-3405.00	kJ/mol	NIST Webbook
chl	-3410.00 ± 0.30	kJ/mol	NIST Webbook
chl	-3418.30 ± 2.10	kJ/mol	NIST Webbook
chl	-3419.00 ± 1.00	kJ/mol	NIST Webbook
gf	-246.21	kJ/mol	Joback Method
hf	-427.71	kJ/mol	Joback Method
hfl	-538.00 ± 1.00	kJ/mol	NIST Webbook
hfus	18.28	kJ/mol	Joback Method
hvap	41.00	kJ/mol	NIST Webbook
log10ws	-1.35		Crippen Method
logp	1.568		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	1007.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1001.40		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	986.00		NIST Webbook

ripol	1510.00		NIST Webbook
ripol	1508.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1466.00		NIST Webbook
ripol	1472.00		NIST Webbook
ripol	1534.00		NIST Webbook
tb	456.20	K	NIST Webbook
tc	634.77	K	Joback Method
tf	259.46	K	Joback Method
vc	0.445	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.90	J/molxK	450.40	Joback Method
cpg	269.47	J/molxK	604.04	Joback Method
cpg	261.25	J/molxK	573.31	Joback Method
cpg	252.68	J/molxK	542.58	Joback Method
cpg	243.77	J/molxK	511.86	Joback Method
cpg	234.51	J/molxK	481.13	Joback Method
cpg	277.34	J/molxK	634.77	Joback Method
dvisc	0.0003003	Paxs	450.40	Joback Method
dvisc	0.0003813	Paxs	418.58	Joback Method
dvisc	0.0005036	Paxs	386.75	Joback Method
dvisc	0.0006992	Paxs	354.93	Joback Method
dvisc	0.0010354	Paxs	323.11	Joback Method
dvisc	0.0016707	Paxs	291.28	Joback Method
dvisc	0.0030315	Paxs	259.46	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.00	K	2.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C590023&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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