Propanoic acid, 2,3-dichloro-, butyl ester

Other names: Propanoic acid, 2,3-dichloro-, butyl ester
butyl 2,3-dichloropropionate
Inchi: InChI=1S/C7H12Cl2O2/c1-2-3-4-11-7(10)6(9)5-8/h6H,2-5H2,1H3
InchiKey: RQSDGSZMJSYKBB-UHFFFAOYSA-N
Formula: C7H12Cl2O2
SMILES: CCCCOC(=O)C(Cl)CCl
Mol. weight [g/mol]: 199.08

Physical Properties

Property code	Value	Unit	Source
af	0.5174		Cheméo Relay (1.0)
hf	-575.64	kJ/mol	Cheméo Relay (1.0)
hfus	21.54	kJ/mol	Joback Method
hvap	56.36	kJ/mol	Cheméo Relay (1.0)
ie	10.50	eV	Cheméo Relay (1.0)
log10ws	-2.48		Cheméo Relay (1.0)
logp	2.176		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1184.00		NIST Webbook
rinpol	1184.00		NIST Webbook
ripol	1669.00		NIST Webbook
tb	475.39	K	Cheméo Relay (1.0)
tc	682.64	K	Cheméo Relay (1.0)
tf	251.71	K	Cheméo Relay (1.0)
vc	0.509	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.96	J/mol×K	510.27	Joback Method
cpg	301.62	J/mol×K	542.29	Joback Method
cpg	311.82	J/mol×K	574.32	Joback Method
cpg	321.54	J/mol×K	606.34	Joback Method

cpg	330.81	J/mol×K	638.37	Joback Method
cpg	339.62	J/mol×K	670.39	Joback Method
cpg	347.98	J/mol×K	702.42	Joback Method
dvisc	0.0037541	Pa×s	285.65	Joback Method
dvisc	0.0018698	Pa×s	323.09	Joback Method
dvisc	0.0010763	Pa×s	360.52	Joback Method
dvisc	0.0006874	Pa×s	397.96	Joback Method
dvisc	0.0004742	Pa×s	435.40	Joback Method
dvisc	0.0003470	Pa×s	472.83	Joback Method
dvisc	0.0002658	Pa×s	510.27	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72726182&Units=SI
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):

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