Butanoic acid, 2,2-dichloro-, methyl ester

Other names: Butyric acid, 2,2-dichloro-, methyl ester
Inchi: InChI=1S/C5H8Cl2O2/c1-3-5(6,7)4(8)9-2/h3H2,1-2H3
InchiKey: VAPJFYJBCCPOAV-UHFFFAOYSA-N
Formula: C5H8Cl2O2
SMILES: CCC(Cl)(Cl)C(=O)OC
Mol. weight [g/mol]: 171.02
CAS: 18545-44-3

Physical Properties

Property code	Value	Unit	Source
gf	-263.72	kJ/mol	Joback Method
hf	-431.56	kJ/mol	Joback Method
hfus	12.47	kJ/mol	Joback Method
hvap	43.35	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.743		Crippen Method
mcvol	113.230	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	957.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	957.00		NIST Webbook
rinpol	949.00		NIST Webbook
tb	461.72	K	Joback Method
tc	666.97	K	Joback Method
tf	280.53	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.59	J/mol×K	461.72	Joback Method
cpg	221.52	J/mol×K	495.93	Joback Method
cpg	229.94	J/mol×K	530.14	Joback Method
cpg	237.86	J/mol×K	564.34	Joback Method

cpg	245.30	J/mol×K	598.55	Joback Method
cpg	252.27	J/mol×K	632.76	Joback Method
cpg	258.80	J/mol×K	666.97	Joback Method
dvisc	0.0037813	Pa×s	280.53	Joback Method
dvisc	0.0020747	Pa×s	310.73	Joback Method
dvisc	0.0012660	Pa×s	340.93	Joback Method
dvisc	0.0008372	Pa×s	371.12	Joback Method
dvisc	0.0005892	Pa×s	401.32	Joback Method
dvisc	0.0004356	Pa×s	431.52	Joback Method
dvisc	0.0003350	Pa×s	461.72	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=C18545443&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: 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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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