Dichloroacetic acid, 2-butyl ester

Other names: Acetic acid, dichloro, 1-methylpropyl ester
Inchi: InChI=1S/C6H10Cl2O2/c1-3-4(2)10-6(9)5(7)8/h4-5H,3H2,1-2H3
InchiKey: IQYVZHJFEAIITM-UHFFFAOYSA-N
Formula: C6H10Cl2O2
SMILES: CCC(C)OC(=O)C(Cl)Cl
Mol. weight [g/mol]: 185.05
CAS: 62223-12-5

Physical Properties

Property code	Value	Unit	Source
gf	-263.02	kJ/mol	Joback Method
hf	-454.01	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	46.10	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.132		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	1015.00		NIST Webbook
ripol	1427.00		NIST Webbook
tb	486.95	K	Joback Method
tc	685.84	K	Joback Method
tf	259.38	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.45	J/mol×K	486.95	Joback Method
cpg	294.25	J/mol×K	652.69	Joback Method
cpg	286.16	J/mol×K	619.54	Joback Method
cpg	277.63	J/mol×K	586.39	Joback Method
cpg	268.68	J/mol×K	553.25	Joback Method
cpg	259.28	J/mol×K	520.10	Joback Method

cpg	301.92	J/mol×K	685.84	Joback Method
dvisc	0.0002759	Pa×s	486.95	Joback Method
dvisc	0.0003681	Pa×s	449.02	Joback Method
dvisc	0.0005180	Pa×s	411.09	Joback Method
dvisc	0.0007812	Pa×s	373.16	Joback Method
dvisc	0.0012930	Pa×s	335.24	Joback Method
dvisc	0.0024337	Pa×s	297.31	Joback Method
dvisc	0.0055114	Pa×s	259.38	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=C62223125&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume