Dichloroacetic acid 3-methylbutyl ester

Other names: Acetic acid, dichloro, 3-methylbutyl ester
Isopentyl dichloroacetate
Inchi: InChI=1S/C7H12Cl2O2/c1-5(2)3-4-11-7(10)6(8)9/h5-6H,3-4H2,1-2H3
InchiKey: UQQSGXRKRFDREY-UHFFFAOYSA-N
Formula: C7H12Cl2O2
SMILES: CC(C)CCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 199.07
CAS: 37587-83-0

Physical Properties

Property code	Value	Unit	Source
chl	-3941.70 ± 8.40	kJ/mol	NIST Webbook
chl	-3932.00	kJ/mol	NIST Webbook
gf	-254.60	kJ/mol	Joback Method
hf	-519.70 ± 9.60	kJ/mol	NIST Webbook
hfl	-575.30 ± 8.40	kJ/mol	NIST Webbook
hfus	18.02	kJ/mol	Joback Method
hvap	55.60 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.29		Crippen Method
logp	2.379		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1129.60		NIST Webbook
ripol	1567.00		NIST Webbook
ripol	1567.00		NIST Webbook
tb	509.83	K	Joback Method
tc	706.13	K	Joback Method
tf	270.65	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.25	J/mol×K	509.83	Joback Method
cpg	302.21	J/mol×K	542.55	Joback Method
cpg	312.68	J/mol×K	575.26	Joback Method
cpg	322.65	J/mol×K	607.98	Joback Method
cpg	332.13	J/mol×K	640.70	Joback Method
cpg	341.13	J/mol×K	673.41	Joback Method
cpg	349.65	J/mol×K	706.13	Joback Method
dvisc	0.0052697	Pa×s	270.65	Joback Method
dvisc	0.0022910	Pa×s	310.51	Joback Method
dvisc	0.0012039	Pa×s	350.38	Joback Method
dvisc	0.0007215	Pa×s	390.24	Joback Method
dvisc	0.0004754	Pa×s	430.10	Joback Method
dvisc	0.0003363	Pa×s	469.97	Joback Method
dvisc	0.0002511	Pa×s	509.83	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37587830&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume