Dichloroacetic acid, allyl ester

Other names:	Allyl dichloroacetate
	2-Propen-1-ol, dichloroacetate
Inchi:	InChI=1S/C5H6Cl2O2/c1-2-3-9-5(8)4(6)7/h2,4H,1,3H2
InchiKey:	UJUPTENXDPFFDP-UHFFFAOYSA-N
Formula:	C5H6Cl2O2
SMILES:	C=CCOC(=O)C(Cl)Cl
Mol. weight [g/mol]:	169.01
CAS:	30895-77-3

Physical Properties

Property code	Value	Unit	Source
chl	-2925.00 ± 3.00	kJ/mol	NIST Webbook
chl	-2479.00	kJ/mol	NIST Webbook
gf	-181.16	kJ/mol	Joback Method
hf	-302.66	kJ/mol	Joback Method
hfus	15.08	kJ/mol	Joback Method
hvap	43.59	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.519		Crippen Method
mcvol	108.930	ml/mol	McGowan Method
pc	3560.02	kPa	Joback Method
rinpol	946.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	946.00		NIST Webbook
ripol	1504.00		NIST Webbook
tb	461.19	K	Joback Method
tc	662.38	K	Joback Method
tf	261.35	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.30	J/mol×K	461.19	Joback Method

cpg	227.24	J/mol×K	628.85	Joback Method
cpg	221.14	J/mol×K	595.32	Joback Method
cpg	214.70	J/mol×K	561.79	Joback Method
cpg	207.92	J/mol×K	528.25	Joback Method
cpg	200.79	J/mol×K	494.72	Joback Method
cpg	233.00	J/mol×K	662.38	Joback Method
dvisc	0.0003182	Pa×s	461.19	Joback Method
dvisc	0.0004074	Pa×s	427.88	Joback Method
dvisc	0.0005439	Pa×s	394.58	Joback Method
dvisc	0.0007659	Pa×s	361.27	Joback Method
dvisc	0.0011562	Pa×s	327.96	Joback Method
dvisc	0.0019155	Pa×s	294.66	Joback Method
dvisc	0.0036093	Pa×s	261.35	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=C30895773&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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

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