Dichloroacetic anhydride

Other names:	Dichloroacetetic anhydride
	Acetic acid, dichloro-, anhydride
	Dichloroacetic acid anhydride
	Anhydrid kyseliny dichloroctove
	2,2'-dichloroacetic anhydride
Inchi:	InChI=1S/C4H2Cl4O3/c5-1(6)3(9)11-4(10)2(7)8/h1-2H
InchiKey:	RQHMQURGSQBBJY-UHFFFAOYSA-N
Formula:	C4H2Cl4O3
SMILES:	O=C(OC(=O)C(Cl)Cl)C(Cl)Cl
Mol. weight [g/mol]:	239.87
CAS:	4124-30-5

Physical Properties

Property code	Value	Unit	Source
gf	-432.64	kJ/mol	Joback Method
hf	-556.79	kJ/mol	Joback Method
hfus	20.24	kJ/mol	Joback Method
hvap	57.16	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.664		Crippen Method
mcvol	125.190	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
rinpol	1248.00		NIST Webbook
tb	488.20	K	NIST Webbook
tc	794.15	K	Joback Method
tf	346.61	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.09	J/mol×K	569.92	Joback Method
cpg	222.51	J/mol×K	607.29	Joback Method
cpg	227.55	J/mol×K	644.66	Joback Method

cpg	232.21	J/mol×K	682.04	Joback Method
cpg	236.49	J/mol×K	719.41	Joback Method
cpg	240.39	J/mol×K	756.78	Joback Method
cpg	243.90	J/mol×K	794.15	Joback Method
dvisc	0.0032164	Pa×s	346.61	Joback Method
dvisc	0.0018063	Pa×s	383.83	Joback Method
dvisc	0.0011233	Pa×s	421.05	Joback Method
dvisc	0.0007546	Pa×s	458.27	Joback Method
dvisc	0.0005382	Pa×s	495.48	Joback Method
dvisc	0.0004023	Pa×s	532.70	Joback Method
dvisc	0.0003125	Pa×s	569.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4124305&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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