

Dichloroacetic anhydride

Other names:	Dichloroacetic 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:	RQHMQRGSQB BJY-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
mvol	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	m ³ /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/molxK	682.04	Joback Method
cpg	236.49	J/molxK	719.41	Joback Method
cpg	240.39	J/molxK	756.78	Joback Method
cpg	243.90	J/molxK	794.15	Joback Method
dvisc	0.0032164	Paxs	346.61	Joback Method
dvisc	0.0018063	Paxs	383.83	Joback Method
dvisc	0.0011233	Paxs	421.05	Joback Method
dvisc	0.0007546	Paxs	458.27	Joback Method
dvisc	0.0005382	Paxs	495.48	Joback Method
dvisc	0.0004023	Paxs	532.70	Joback Method
dvisc	0.0003125	Paxs	569.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4124305&Units=SI

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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