

1,1,2-Trichloropropanoic anhydride

Inchi:	InChI=1S/C6H4Cl6O3/c7-1-5(9,10)3(13)15-4(14)6(11,12)2-8/h1-2H2
InchiKey:	SUGRZHYYBAXPPQ-UHFFFAOYSA-N
Formula:	C6H4Cl6O3
SMILES:	O=C(OC(=O)C(Cl)(Cl)CCl)C(Cl)(Cl)CCl
Mol. weight [g/mol]:	336.81
CAS:	116402-54-1

Physical Properties

Property code	Value	Unit	Source
gf	-429.10	kJ/mol	Joback Method
hf	-636.49	kJ/mol	Joback Method
hfus	26.04	kJ/mol	Joback Method
hvap	68.57	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.882		Crippen Method
mcvol	177.850	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
tb	684.96	K	Joback Method
tc	924.49	K	Joback Method
tf	463.83	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.23	J/molxK	684.96	Joback Method
cpg	352.16	J/molxK	724.88	Joback Method
cpg	357.40	J/molxK	764.80	Joback Method
cpg	362.02	J/molxK	804.72	Joback Method
cpg	366.09	J/molxK	844.65	Joback Method
cpg	369.67	J/molxK	884.57	Joback Method
cpg	372.84	J/molxK	924.49	Joback Method
dvisc	0.0012671	Paxs	463.83	Joback Method
dvisc	0.0007873	Paxs	500.69	Joback Method

dvisc	0.0005221	Paxs	537.54	Joback Method
dvisc	0.0003650	Paxs	574.39	Joback Method
dvisc	0.0002664	Paxs	611.25	Joback Method
dvisc	0.0002016	Paxs	648.11	Joback Method
dvisc	0.0001572	Paxs	684.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402541&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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