

Tribromoacetic acid

Other names:	Tribromacetic acid Acetic acid, tribromo-
Inchi:	InChI=1S/C2HBr3O2/c3-2(4,5)1(6)7/h(H,6,7)
InchiKey:	QIONYIKHPASLHO-UHFFFAOYSA-N
Formula:	C2HBr3O2
SMILES:	O=C(O)C(Br)(Br)Br
Mol. weight [g/mol]:	296.74
CAS:	75-96-7

Physical Properties

Property code	Value	Unit	Source
gf	-253.98	kJ/mol	Joback Method
hf	-279.18	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	61.48	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.909		Crippen Method
mvol	98.980	ml/mol	McGowan Method
pc	9444.29	kPa	Joback Method
tb	518.20	K	NIST Webbook
tc	823.73	K	Joback Method
tf	404.87	K	Joback Method
vc	0.347	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.79	J/molxK	586.46	Joback Method
cpg	146.24	J/molxK	626.00	Joback Method
cpg	148.27	J/molxK	665.55	Joback Method
cpg	149.97	J/molxK	705.09	Joback Method
cpg	151.40	J/molxK	744.64	Joback Method
cpg	152.63	J/molxK	784.18	Joback Method
cpg	153.73	J/molxK	823.73	Joback Method

dvisc	0.0026542	Paxs	404.87	Joback Method
dvisc	0.0014400	Paxs	435.13	Joback Method
dvisc	0.0008459	Paxs	465.40	Joback Method
dvisc	0.0005303	Paxs	495.67	Joback Method
dvisc	0.0003508	Paxs	525.93	Joback Method
dvisc	0.0002427	Paxs	556.20	Joback Method
dvisc	0.0001745	Paxs	586.46	Joback Method

Sources

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=C75967&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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