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

Physical Properties

Property code	Value	Unit	Source
hf	-265.63	kJ/mol	Cheméo Relay (1.0)
hfus	15.06	kJ/mol	Joback Method
hvap	66.21	kJ/mol	Cheméo Relay (1.0)
ie	11.08	eV	Cheméo Relay (1.0)
logp	1.909		Crippen Method
mcvol	98.980	ml/mol	McGowan Method
tb	518.20	K	NIST Webbook
tf	332.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.79	J/mol×K	586.46	Joback Method
cpg	153.73	J/mol×K	823.73	Joback Method
cpg	152.63	J/mol×K	784.18	Joback Method
cpg	151.40	J/mol×K	744.64	Joback Method
cpg	149.97	J/mol×K	705.09	Joback Method
cpg	148.27	J/mol×K	665.55	Joback Method
cpg	146.24	J/mol×K	626.00	Joback Method
dvisc	0.0005303	Pa×s	495.67	Joback Method
dvisc	0.0001745	Pa×s	586.46	Joback Method
dvisc	0.0002427	Pa×s	556.20	Joback Method
dvisc	0.0003508	Pa×s	525.93	Joback Method
dvisc	0.0026542	Pa×s	404.87	Joback Method

dvisc	0.0008459	Pa×s	465.40	Joback Method
dvisc	0.0014400	Pa×s	435.13	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75967&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point