

2,2,2-tribromoethane-1,1-diol

Inchi:	InChI=1S/C2H3Br3O2/c3-2(4,5)1(6)7/h1,6-7H
InchiKey:	NJHVVMXFNIZTTBV-UHFFFAOYSA-N
Formula:	C2H3Br3O2
SMILES:	OC(O)C(Br)(Br)Br
Mol. weight [g/mol]:	298.76
CAS:	507-42-6

Physical Properties

Property code	Value	Unit	Source
gf	-264.32	kJ/mol	Joback Method
hf	-324.11	kJ/mol	Joback Method
hfus	14.03	kJ/mol	Joback Method
hvap	71.03	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.136		Crippen Method
mcvol	103.280	ml/mol	McGowan Method
pc	10161.94	kPa	Joback Method
tb	624.33	K	Joback Method
tc	840.05	K	Joback Method
tf	319.15 ± 0.70	K	NIST Webbook
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.86	J/molxK	624.33	Joback Method
cpg	171.59	J/molxK	660.28	Joback Method
cpg	173.98	J/molxK	696.24	Joback Method
cpg	176.10	J/molxK	732.19	Joback Method
cpg	178.01	J/molxK	768.15	Joback Method
cpg	179.76	J/molxK	804.10	Joback Method
cpg	181.42	J/molxK	840.05	Joback Method
dvisc	0.0037582	Paxs	400.76	Joback Method
dvisc	0.0012810	Paxs	438.02	Joback Method

dvisc	0.0005169	Paxs	475.28	Joback Method
dvisc	0.0002380	Paxs	512.54	Joback Method
dvisc	0.0001217	Paxs	549.81	Joback Method
dvisc	0.0000678	Paxs	587.07	Joback Method
dvisc	0.0000405	Paxs	624.33	Joback Method

Sources

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=C507426&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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