

# Acetic acid, tribromo, 1,2-dimethylpropyl ester

<b>Inchi:</b>	InChI=1S/C7H11Br3O2/c1-4(2)5(3)12-6(11)7(8,9)10/h4-5H,1-3H3
<b>InchiKey:</b>	AIOAXQWRROPLIL-UHFFFAOYSA-N
<b>Formula:</b>	C7H11Br3O2
<b>SMILES:</b>	CC(C)C(C)OC(=O)C(Br)(Br)Br
<b>Mol. weight [g/mol]:</b>	366.87

## Physical Properties

Property code	Value	Unit	Source
gf	-184.94	kJ/mol	Joback Method
hf	-372.93	kJ/mol	Joback Method
hfus	18.07	kJ/mol	Joback Method
hvap	57.56	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.413		Crippen Method
mcvol	169.430	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
rinpol	1446.00		NIST Webbook
tb	630.22	K	Joback Method
tc	871.47	K	Joback Method
tf	392.63	K	Joback Method
vc	0.615	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.40	J/molxK	630.22	Joback Method
cpg	391.97	J/molxK	831.26	Joback Method
cpg	384.62	J/molxK	791.05	Joback Method
cpg	376.66	J/molxK	750.84	Joback Method
cpg	368.02	J/molxK	710.64	Joback Method
cpg	358.62	J/molxK	670.43	Joback Method
cpg	398.78	J/molxK	871.47	Joback Method
dvisc	0.0001764	Paxs	630.22	Joback Method
dvisc	0.0002303	Paxs	590.62	Joback Method

dvisc	0.0003125	Paxs	551.02	Joback Method
dvisc	0.0004446	Paxs	511.43	Joback Method
dvisc	0.0006710	Paxs	471.83	Joback Method
dvisc	0.0010921	Paxs	432.23	Joback Method
dvisc	0.0019609	Paxs	392.63	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R115792&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R115792&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/25-976-1/Acetic-acid-tribromo-1-2-dimethylpropyl-ester.pdf>

Generated by Cheméo on 2024-05-01 02:40:00.679079792 +0000 UTC m=+16820449.599657102.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.