

Acetic acid, tribromo, 1-methylbutyl ester

Inchi:	InChI=1S/C7H11Br3O2/c1-3-4-5(2)12-6(11)7(8,9)10/h5H,3-4H2,1-2H3
InchiKey:	MJLVEJKVDIYJEE-UHFFFAOYSA-N
Formula:	C7H11Br3O2
SMILES:	CCCC(C)OC(=O)C(Br)(Br)Br
Mol. weight [g/mol]:	366.87

Physical Properties

Property code	Value	Unit	Source
gf	-182.50	kJ/mol	Joback Method
hf	-367.65	kJ/mol	Joback Method
hfus	21.59	kJ/mol	Joback Method
hvap	57.95	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.557		Crippen Method
mvol	169.430	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
rinpol	1458.00		NIST Webbook
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tb	630.66	K	Joback Method
tc	866.79	K	Joback Method
tf	407.63	K	Joback Method
vc	0.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.87	J/molxK	630.66	Joback Method
cpg	390.55	J/molxK	827.43	Joback Method
cpg	383.30	J/molxK	788.08	Joback Method
cpg	375.48	J/molxK	748.72	Joback Method
cpg	367.01	J/molxK	709.37	Joback Method
cpg	357.83	J/molxK	670.01	Joback Method
cpg	397.29	J/molxK	866.79	Joback Method
dvisc	0.0001894	Paxs	630.66	Joback Method

dvisc	0.0002421	Paxs	593.49	Joback Method
dvisc	0.0003197	Paxs	556.32	Joback Method
dvisc	0.0004394	Paxs	519.14	Joback Method
dvisc	0.0006342	Paxs	481.97	Joback Method
dvisc	0.0009734	Paxs	444.80	Joback Method
dvisc	0.0016153	Paxs	407.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R115801&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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