Acetic acid, tribromo, 3-methylbutyl ester

Inchi: InChI=1S/C7H11Br3O2/c1-5(2)3-4-12-6(11)7(8,9)10/h5H,3-4H2,1-2H3
InchiKey: MQOMZSFUDDSYJF-UHFFFAOYSA-N
Formula: C7H11Br3O2
SMILES: CC(C)CCOC(=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	-3.77		Crippen Method
logp	3.414		Crippen Method
mcvol	169.430	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
rinpol	1492.00		NIST Webbook
rinpol	1492.00		NIST Webbook
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/mol×K	630.66	Joback Method
cpg	357.83	J/mol×K	670.01	Joback Method
cpg	367.01	J/mol×K	709.37	Joback Method
cpg	375.48	J/mol×K	748.72	Joback Method
cpg	383.30	J/mol×K	788.08	Joback Method
cpg	390.55	J/mol×K	827.43	Joback Method
cpg	397.29	J/mol×K	866.79	Joback Method
dvisc	0.0016153	Pa×s	407.63	Joback Method

dvisc	0.0009734	Pa×s	444.80	Joback Method
dvisc	0.0006342	Pa×s	481.97	Joback Method
dvisc	0.0004394	Pa×s	519.14	Joback Method
dvisc	0.0003197	Pa×s	556.32	Joback Method
dvisc	0.0002421	Pa×s	593.49	Joback Method
dvisc	0.0001894	Pa×s	630.66	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=R115836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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