Acetic acid, tribromo, 1-methylpropyl ester

Inchi: InChI=1S/C6H9Br3O2/c1-3-4(2)11-5(10)6(7,8)9/h4H,3H2,1-2H3
InchiKey: OLNZDRWZSBAEIJ-UHFFFAOYSA-N
Formula: C6H9Br3O2
SMILES: CCC(C)OC(=O)C(Br)(Br)Br
Mol. weight [g/mol]: 352.85

Physical Properties

Property code	Value	Unit	Source
gf	-190.92	kJ/mol	Joback Method
hf	-347.01	kJ/mol	Joback Method
hfus	19.00	kJ/mol	Joback Method
hvap	55.73	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.167		Crippen Method
mcvol	155.340	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
rinpol	1366.00		NIST Webbook
tb	607.78	K	Joback Method
tc	848.93	K	Joback Method
tf	396.36	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.29	J/mol×K	607.78	Joback Method
cpg	311.30	J/mol×K	647.97	Joback Method
cpg	319.57	J/mol×K	688.16	Joback Method
cpg	327.15	J/mol×K	728.36	Joback Method
cpg	334.12	J/mol×K	768.55	Joback Method
cpg	340.54	J/mol×K	808.74	Joback Method
cpg	346.48	J/mol×K	848.93	Joback Method
dvisc	0.0017759	Pa×s	396.36	Joback Method
dvisc	0.0010885	Pa×s	431.60	Joback Method

dvisc	0.0007184	Pa×s	466.83	Joback Method
dvisc	0.0005026	Pa×s	502.07	Joback Method
dvisc	0.0003685	Pa×s	537.31	Joback Method
dvisc	0.0002807	Pa×s	572.54	Joback Method
dvisc	0.0002206	Pa×s	607.78	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=R115816&Units=SI

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