Acetic acid, dibromo, 1,1-dimethylpropyl ester

Inchi: InChI=1S/C7H12Br2O2/c1-4-7(2,3)11-6(10)5(8)9/h5H,4H2,1-3H3
InchiKey: PAVSJRNSWFMTBQ-UHFFFAOYSA-N
Formula: C7H12Br2O2
SMILES: CCC(C)(C)OC(=O)C(Br)Br
Mol. weight [g/mol]: 287.98

Physical Properties

Property code	Value	Unit	Source
gf	-196.82	kJ/mol	Joback Method
hf	-393.98	kJ/mol	Joback Method
hfus	16.31	kJ/mol	Joback Method
hvap	51.52	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.834		Crippen Method
mcvol	151.930	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	1221.00		NIST Webbook
ripol	1680.00		NIST Webbook
tb	564.50	K	Joback Method
tc	787.92	K	Joback Method
tf	347.83	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.07	J/mol×K	564.50	Joback Method
cpg	327.27	J/mol×K	601.74	Joback Method
cpg	337.71	J/mol×K	638.97	Joback Method
cpg	347.42	J/mol×K	676.21	Joback Method
cpg	356.44	J/mol×K	713.45	Joback Method
cpg	364.84	J/mol×K	750.68	Joback Method
cpg	372.65	J/mol×K	787.92	Joback Method
dvisc	0.0026608	Pa×s	347.83	Joback Method

dvisc	0.0014734	Pa×s	383.94	Joback Method
dvisc	0.0009032	Pa×s	420.05	Joback Method
dvisc	0.0005982	Pa×s	456.17	Joback Method
dvisc	0.0004209	Pa×s	492.28	Joback Method
dvisc	0.0003108	Pa×s	528.39	Joback Method
dvisc	0.0002385	Pa×s	564.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R115643&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume