Acetic acid, dibromo, 1,2-dimethylpropyl ester

Inchi: InChI=1S/C7H12Br2O2/c1-4(2)5(3)11-7(10)6(8)9/h4-6H,1-3H3
InchiKey: CEXIVSAQDYUXAN-UHFFFAOYSA-N
Formula: C7H12Br2O2
SMILES: CC(C)C(C)OC(=O)C(Br)Br
Mol. weight [g/mol]: 287.98

Physical Properties

Property code	Value	Unit	Source
gf	-204.54	kJ/mol	Joback Method
hf	-395.79	kJ/mol	Joback Method
hfus	16.67	kJ/mol	Joback Method
hvap	52.04	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.690		Crippen Method
mcvol	151.930	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
rinpol	1244.00		NIST Webbook
ripol	1717.00		NIST Webbook
tb	566.85	K	Joback Method
tc	786.25	K	Joback Method
tf	315.41	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.16	J/mol×K	566.85	Joback Method
cpg	324.29	J/mol×K	603.42	Joback Method
cpg	334.77	J/mol×K	639.98	Joback Method
cpg	344.62	J/mol×K	676.55	Joback Method
cpg	353.86	J/mol×K	713.12	Joback Method
cpg	362.51	J/mol×K	749.68	Joback Method
cpg	370.60	J/mol×K	786.25	Joback Method
dvisc	0.0039264	Pa×s	315.41	Joback Method

dvisc	0.0018521	Pa×s	357.32	Joback Method
dvisc	0.0010229	Pa×s	399.22	Joback Method
dvisc	0.0006324	Pa×s	441.13	Joback Method
dvisc	0.0004250	Pa×s	483.04	Joback Method
dvisc	0.0003043	Pa×s	524.94	Joback Method
dvisc	0.0002289	Pa×s	566.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R115658&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume