Acetic acid, dibromo, 2-methylpropyl ester

Inchi: InChI=1S/C6H10Br2O2/c1-4(2)3-10-6(9)5(7)8/h4-5H,3H2,1-2H3
InchiKey: FJDHOUKYKISYRM-UHFFFAOYSA-N
Formula: C6H10Br2O2
SMILES: CC(C)COC(=O)C(Br)Br
Mol. weight [g/mol]: 273.95

Physical Properties

Property code	Value	Unit	Source
gf	-210.52	kJ/mol	Joback Method
hf	-369.87	kJ/mol	Joback Method
hfus	17.61	kJ/mol	Joback Method
hvap	50.20	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.301		Crippen Method
mcvol	137.840	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
rinpol	1187.00		NIST Webbook
rinpol	1187.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1701.00		NIST Webbook
tb	544.41	K	Joback Method
tc	762.87	K	Joback Method
tf	319.14	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.87	J/mol×K	544.41	Joback Method
cpg	278.66	J/mol×K	580.82	Joback Method
cpg	287.88	J/mol×K	617.23	Joback Method
cpg	296.57	J/mol×K	653.64	Joback Method
cpg	304.73	J/mol×K	690.05	Joback Method
cpg	312.38	J/mol×K	726.46	Joback Method

cpg	319.55	J/mol×K	762.87	Joback Method
dvisc	0.0031975	Pa×s	319.14	Joback Method
dvisc	0.0017149	Pa×s	356.69	Joback Method
dvisc	0.0010356	Pa×s	394.23	Joback Method
dvisc	0.0006828	Pa×s	431.77	Joback Method
dvisc	0.0004812	Pa×s	469.32	Joback Method
dvisc	0.0003571	Pa×s	506.86	Joback Method
dvisc	0.0002762	Pa×s	544.41	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=R115698&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume