Acetic acid, dibromo, 1-methylpropyl ester

Inchi: InChI=1S/C6H10Br2O2/c1-3-4(2)10-6(9)5(7)8/h4-5H,3H2,1-2H3
InchiKey: PNWWZNZTEYSBAW-UHFFFAOYSA-N
Formula: C6H10Br2O2
SMILES: CCC(C)OC(=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	-2.78		Crippen Method
logp	2.444		Crippen Method
mcvol	137.840	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
rinpol	1169.00		NIST Webbook
rinpol	1169.00		NIST Webbook
ripol	1663.00		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=R115683&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

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