Acetic acid, dibromo, 1,1-dimethylethyl ester

Inchi: InChI=1S/C6H10Br2O2/c1-6(2,3)10-5(9)4(7)8/h4H,1-3H3
InchiKey: WVNZGIJOOOHIPU-UHFFFAOYSA-N
Formula: C6H10Br2O2
SMILES: CC(C)(C)OC(=O)C(Br)Br
Mol. weight [g/mol]: 273.95

Physical Properties

Property code	Value	Unit	Source
gf	-205.24	kJ/mol	Joback Method
hf	-373.34	kJ/mol	Joback Method
hfus	13.72	kJ/mol	Joback Method
hvap	49.29	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.444		Crippen Method
mcvol	137.840	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	1103.00		NIST Webbook
rinpol	1103.00		NIST Webbook
ripol	1564.00		NIST Webbook
tb	541.62	K	Joback Method
tc	769.22	K	Joback Method
tf	336.56	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.30	J/mol×K	541.62	Joback Method
cpg	282.50	J/mol×K	579.55	Joback Method
cpg	291.97	J/mol×K	617.49	Joback Method
cpg	300.75	J/mol×K	655.42	Joback Method
cpg	308.88	J/mol×K	693.36	Joback Method
cpg	316.42	J/mol×K	731.29	Joback Method
cpg	323.40	J/mol×K	769.22	Joback Method

dvisc	0.0028816	Pa×s	336.56	Joback Method
dvisc	0.0016249	Pa×s	370.74	Joback Method
dvisc	0.0010093	Pa×s	404.91	Joback Method
dvisc	0.0006752	Pa×s	439.09	Joback Method
dvisc	0.0004786	Pa×s	473.27	Joback Method
dvisc	0.0003554	Pa×s	507.44	Joback Method
dvisc	0.0002740	Pa×s	541.62	Joback Method

Sources

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=R115638&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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