Acetic acid, bromo, 1,1-dimethylpropyl ester

Inchi: InChI=1S/C7H13BrO2/c1-4-7(2,3)10-6(9)5-8/h4-5H2,1-3H3
InchiKey: GNEJWGLFBZOLAE-UHFFFAOYSA-N
Formula: C7H13BrO2
SMILES: CCC(C)(C)OC(=O)CBr
Mol. weight [g/mol]: 209.08

Physical Properties

Property code	Value	Unit	Source
gf	-208.70	kJ/mol	Joback Method
hf	-415.03	kJ/mol	Joback Method
hfus	14.54	kJ/mol	Joback Method
hvap	45.47	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.113		Crippen Method
mcvol	134.430	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	1065.00		NIST Webbook
ripol	1472.00		NIST Webbook
tb	498.78	K	Joback Method
tc	703.02	K	Joback Method
tf	303.03	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.15	J/mol×K	498.78	Joback Method
cpg	332.90	J/mol×K	668.98	Joback Method
cpg	323.58	J/mol×K	634.94	Joback Method
cpg	313.67	J/mol×K	600.90	Joback Method
cpg	303.15	J/mol×K	566.86	Joback Method
cpg	291.98	J/mol×K	532.82	Joback Method
cpg	341.67	J/mol×K	703.02	Joback Method
dvisc	0.0002899	Pa×s	498.78	Joback Method

dvisc	0.0003766	Pa×s	466.15	Joback Method
dvisc	0.0005087	Pa×s	433.53	Joback Method
dvisc	0.0007217	Pa×s	400.90	Joback Method
dvisc	0.0010893	Pa×s	368.28	Joback Method
dvisc	0.0017812	Pa×s	335.66	Joback Method
dvisc	0.0032379	Pa×s	303.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R115574&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