Acetic acid, bromo-, 1,1-dimethylethyl ester

Other names:	BrCH2C(O)OC(CH3)3
	tert-Butyl bromoacetate
	t-Butyl bromoacetate
	Acetic acid, bromo-, tert-butyl ester
Inchi:	InChI=1S/C6H11BrO2/c1-6(2,3)9-5(8)4-7/h4H2,1-3H3
InchiKey:	BNWCETAHAJSBFG-UHFFFAOYSA-N
Formula:	C6H11BrO2
SMILES:	CC(C)(C)OC(=O)CBr
Mol. weight [g/mol]:	195.05
CAS:	5292-43-3

Physical Properties

Property code	Value	Unit	Source
gf	-217.12	kJ/mol	Joback Method
hf	-394.39	kJ/mol	Joback Method
hfus	11.95	kJ/mol	Joback Method
hvap	43.25	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.723		Crippen Method
mcvol	120.340	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	949.00		NIST Webbook
rinpol	949.00		NIST Webbook
ripol	1359.00		NIST Webbook
tb	475.90	K	Joback Method
tc	683.03	K	Joback Method
tf	291.76	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.55	J/mol×K	475.90	Joback Method
cpg	249.29	J/mol×K	510.42	Joback Method

cpg	259.40	J/mol×K	544.94	Joback Method
cpg	268.93	J/mol×K	579.47	Joback Method
cpg	277.88	J/mol×K	613.99	Joback Method
cpg	286.30	J/mol×K	648.51	Joback Method
cpg	294.19	J/mol×K	683.03	Joback Method
dvisc	0.0033846	Pa×s	291.76	Joback Method
dvisc	0.0019006	Pa×s	322.45	Joback Method
dvisc	0.0011798	Pa×s	353.14	Joback Method
dvisc	0.0007905	Pa×s	383.83	Joback Method
dvisc	0.0005619	Pa×s	414.52	Joback Method
dvisc	0.0004187	Pa×s	445.21	Joback Method
dvisc	0.0003241	Pa×s	475.90	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	323.20	K	1.30	NIST Webbook

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=C5292433&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume