Bromoacetic acid, 2-methylpropyl ester

Other names: Bromoacetic acid, 2-methylpropyl ester
Isobutyl bromoacetate
Inchi: InChI=1S/C6H11BrO2/c1-5(2)4-9-6(8)3-7/h5H,3-4H2,1-2H3
InchiKey: UOUQDZFAJUNYQQ-UHFFFAOYSA-N
Formula: C6H11BrO2
SMILES: CC(C)COC(=O)CBr
Mol. weight [g/mol]: 195.06

Physical Properties

Property code	Value	Unit	Source
af	0.5389		Cheméo Relay (1.0)
hf	-485.10	kJ/mol	Cheméo Relay (1.0)
hfus	15.85	kJ/mol	Joback Method
hvap	47.34	kJ/mol	Cheméo Relay (1.0)
ie	10.14	eV	Cheméo Relay (1.0)
log10ws	-1.97		Cheméo Relay (1.0)
logp	1.580		Crippen Method
mcvol	120.340	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
rinpol	1025.80		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1025.80		NIST Webbook
rinpol	1021.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1488.00		NIST Webbook
tb	457.27	K	Cheméo Relay (1.0)
tc	639.61	K	Cheméo Relay (1.0)
tf	249.77	K	Cheméo Relay (1.0)
vc	0.434	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.52	J/mol×K	478.69	Joback Method
cpg	245.58	J/mol×K	511.82	Joback Method
cpg	255.20	J/mol×K	544.95	Joback Method
cpg	264.38	J/mol×K	578.08	Joback Method
cpg	273.13	J/mol×K	611.21	Joback Method
cpg	281.46	J/mol×K	644.34	Joback Method
cpg	289.37	J/mol×K	677.47	Joback Method
dvisc	0.0035442	Pa×s	274.34	Joback Method
dvisc	0.0018866	Pa×s	308.40	Joback Method
dvisc	0.0011385	Pa×s	342.46	Joback Method
dvisc	0.0007528	Pa×s	376.51	Joback Method
dvisc	0.0005331	Pa×s	410.57	Joback Method
dvisc	0.0003980	Pa×s	444.63	Joback Method
dvisc	0.0003098	Pa×s	478.69	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59956488&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
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