Propanoic acid, 2-bromo-2-methyl-, ethyl ester

Other names:	Ethyl «alpha»-bromoisobutyrate
	Ethyl 2-bromoisobutyrate
	Ethyl 2-bromo-2-methylpropionate
	«alpha»-Bromoisobutyric acid, ethyl ester
	Ethyl 2-bromo-2-methylpropanoate
	Propionic acid, 2-bromo-2-methyl-, ethyl ester
	2-Bromo-2-methylpropanoic acid, ethyl ester
	Ethyl «alpha»-bromo-«alpha»-methylpropionate
	NSC 402034
	NSC 9465
Inchi:	InChI=1S/C6H11BrO2/c1-4-9-5(8)6(2,3)7/h4H2,1-3H3
InchiKey:	IOLQWGVDEFWYNP-UHFFFAOYSA-N
Formula:	C6H11BrO2
SMILES:	CCOC(=O)C(C)(C)Br
Mol. weight [g/mol]:	195.05
CAS:	600-00-0

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
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

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C600000&Units=SI

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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