Bromoacetic acid, 2-butyl ester

Other names:	Sec-butyl bromoacetate
	Acetic acid, bromo, 1-mehylpropyl ester
Inchi:	InChI=1S/C6H11BrO2/c1-3-5(2)9-6(8)4-7/h5H,3-4H2,1-2H3
InchiKey:	AYUZHUMAYBBDJY-UHFFFAOYSA-N
Formula:	C6H11BrO2
SMILES:	CCC(C)OC(=O)CBr
Mol. weight [g/mol]:	195.05
CAS:	5205-36-7

Physical Properties

Property code	Value	Unit	Source
gf	-222.40	kJ/mol	Joback Method
hf	-390.92	kJ/mol	Joback Method
hfus	15.85	kJ/mol	Joback Method
hvap	44.15	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.723		Crippen Method
mcvol	120.340	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
rinpol	1006.00		NIST Webbook
ripol	1454.00		NIST Webbook
tb	478.69	K	Joback Method
tc	677.47	K	Joback Method
tf	274.34	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.52	J/mol×K	478.69	Joback Method
cpg	281.46	J/mol×K	644.34	Joback Method
cpg	273.13	J/mol×K	611.21	Joback Method
cpg	264.38	J/mol×K	578.08	Joback Method
cpg	255.20	J/mol×K	544.95	Joback Method

cpg	245.58	J/mol×K	511.82	Joback Method
cpg	289.37	J/mol×K	677.47	Joback Method
dvisc	0.0003098	Pa×s	478.69	Joback Method
dvisc	0.0003980	Pa×s	444.63	Joback Method
dvisc	0.0005331	Pa×s	410.57	Joback Method
dvisc	0.0007528	Pa×s	376.51	Joback Method
dvisc	0.0011385	Pa×s	342.46	Joback Method
dvisc	0.0018866	Pa×s	308.40	Joback Method
dvisc	0.0035442	Pa×s	274.34	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5205367&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

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