3-Buten-1-ol, bromoacetate

Inchi: InChI=1S/C6H9BrO2/c1-2-3-4-9-6(8)5-7/h2H,1,3-5H2
InchiKey: JTGHDLRTHVAJPU-UHFFFAOYSA-N
Formula: C6H9BrO2
SMILES: C=CCCOC(=O)CBr
Mol. weight [g/mol]: 193.04

Physical Properties

Property code	Value	Unit	Source
gf	-132.12	kJ/mol	Joback Method
hf	-260.21	kJ/mol	Joback Method
hfus	18.09	kJ/mol	Joback Method
hvap	43.87	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.501		Crippen Method
mcvol	116.040	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	1040.00		NIST Webbook
rinpol	1040.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1596.00		NIST Webbook
tb	475.81	K	Joback Method
tc	674.35	K	Joback Method
tf	287.58	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.44	J/mol×K	475.81	Joback Method
cpg	227.46	J/mol×K	508.90	Joback Method
cpg	236.05	J/mol×K	541.99	Joback Method
cpg	244.23	J/mol×K	575.08	Joback Method
cpg	252.00	J/mol×K	608.17	Joback Method
cpg	259.38	J/mol×K	641.26	Joback Method

cpg	266.38	J/mol×K	674.35	Joback Method
dvisc	0.0024719	Pa×s	287.58	Joback Method
dvisc	0.0014985	Pa×s	318.95	Joback Method
dvisc	0.0009937	Pa×s	350.32	Joback Method
dvisc	0.0007049	Pa×s	381.70	Joback Method
dvisc	0.0005269	Pa×s	413.07	Joback Method
dvisc	0.0004103	Pa×s	444.44	Joback Method
dvisc	0.0003302	Pa×s	475.81	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=R26407&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
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