Ethanol, 2-bromo-, acetate

Other names:	Bromoethyl acetate
	1-Acetoxy-2-bromoethane
	1-Bromo-2-acetoxyethane
	2-Bromoethyl acetate
Inchi:	InChI=1S/C4H7BrO2/c1-4(6)7-3-2-5/h2-3H2,1H3
InchiKey:	RGHQKFQZGLKBCF-UHFFFAOYSA-N
Formula:	C4H7BrO2
SMILES:	CC(=O)OCCBr
Mol. weight [g/mol]:	167.00
CAS:	927-68-4

Physical Properties

Property code	Value	Unit	Source
gf	-236.80	kJ/mol	Joback Method
hf	-344.36	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	40.09	kJ/mol	Joback Method
log10ws	-0.79		Crippen Method
logp	0.944		Crippen Method
mcvol	92.160	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
rinpol	882.00		NIST Webbook
tb	433.37	K	Joback Method
tc	632.29	K	Joback Method
tf	266.80	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.76	J/mol×K	433.37	Joback Method
cpg	191.30	J/mol×K	599.13	Joback Method
cpg	185.34	J/mol×K	565.98	Joback Method
cpg	179.11	J/mol×K	532.83	Joback Method

cpg	172.60	J/mol×K	499.68	Joback Method
cpg	165.82	J/mol×K	466.52	Joback Method
cpg	196.99	J/mol×K	632.29	Joback Method
dvisc	0.0003772	Pa×s	433.37	Joback Method
dvisc	0.0004662	Pa×s	405.61	Joback Method
dvisc	0.0005942	Pa×s	377.85	Joback Method
dvisc	0.0007873	Pa×s	350.09	Joback Method
dvisc	0.0010947	Pa×s	322.32	Joback Method
dvisc	0.0016199	Pa×s	294.56	Joback Method
dvisc	0.0026007	Pa×s	266.80	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=C927684&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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