7-Bromo-1-heptanol, acetate

Inchi: InChI=1S/C9H17BrO2/c1-9(11)12-8-6-4-2-3-5-7-10/h2-8H2,1H3
InchiKey: YAFBPBCITSMEMS-UHFFFAOYSA-N
Formula: C9H17BrO2
SMILES: CC(=O)OCCCCCCCBr
Mol. weight [g/mol]: 237.13

Physical Properties

Property code	Value	Unit	Source
gf	-194.70	kJ/mol	Joback Method
hf	-447.56	kJ/mol	Joback Method
hfus	27.14	kJ/mol	Joback Method
hvap	51.22	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.895		Crippen Method
mcvol	162.610	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	1477.00		NIST Webbook
rinpol	1477.00		NIST Webbook
tb	547.77	K	Joback Method
tc	735.28	K	Joback Method
tf	323.15	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.76	J/mol×K	547.77	Joback Method
cpg	378.57	J/mol×K	579.02	Joback Method
cpg	390.80	J/mol×K	610.27	Joback Method
cpg	402.47	J/mol×K	641.52	Joback Method
cpg	413.59	J/mol×K	672.78	Joback Method
cpg	424.18	J/mol×K	704.03	Joback Method
cpg	434.25	J/mol×K	735.28	Joback Method
dvisc	0.0024410	Pa×s	323.15	Joback Method

dvisc	0.0013642	Pa×s	360.59	Joback Method
dvisc	0.0008506	Pa×s	398.02	Joback Method
dvisc	0.0005753	Pa×s	435.46	Joback Method
dvisc	0.0004139	Pa×s	472.90	Joback Method
dvisc	0.0003125	Pa×s	510.33	Joback Method
dvisc	0.0002452	Pa×s	547.77	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=U374861&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