4-Penten-2-ol, bromoacetate

Inchi: InChI=1S/C7H11BrO2/c1-3-4-6(2)10-7(9)5-8/h3,6H,1,4-5H2,2H3
InchiKey: CJFYOQXFISOMFE-UHFFFAOYSA-N
Formula: C7H11BrO2
SMILES: C=CCC(C)OC(=O)CBr
Mol. weight [g/mol]: 207.06

Physical Properties

Property code	Value	Unit	Source
gf	-126.14	kJ/mol	Joback Method
hf	-286.13	kJ/mol	Joback Method
hfus	17.16	kJ/mol	Joback Method
hvap	45.71	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.889		Crippen Method
mcvol	130.130	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1076.00		NIST Webbook
ripol	1575.00		NIST Webbook
tb	498.25	K	Joback Method
tc	698.62	K	Joback Method
tf	283.85	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.41	J/mol×K	498.25	Joback Method
cpg	269.90	J/mol×K	531.65	Joback Method
cpg	279.89	J/mol×K	565.04	Joback Method
cpg	289.37	J/mol×K	598.44	Joback Method
cpg	298.37	J/mol×K	631.83	Joback Method
cpg	306.90	J/mol×K	665.23	Joback Method
cpg	314.96	J/mol×K	698.62	Joback Method
dvisc	0.0032347	Pa×s	283.85	Joback Method

dvisc	0.0017256	Pa×s	319.58	Joback Method
dvisc	0.0010445	Pa×s	355.32	Joback Method
dvisc	0.0006930	Pa×s	391.05	Joback Method
dvisc	0.0004925	Pa×s	426.78	Joback Method
dvisc	0.0003690	Pa×s	462.52	Joback Method
dvisc	0.0002881	Pa×s	498.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26532&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

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