Cyclopentanol,2-bromo-,acetate,trans-

Inchi: InChI=1S/C7H11BrO2/c1-5(9)10-7-4-2-3-6(7)8/h6-7H,2-4H2,1H3/t6-,7-/m1/s1
InchiKey: RWFKZZAXUPSAQT-RNFRBKRXSA-N
Formula: C7H11BrO2
SMILES: CC(=O)OC1CCCC1Br
Mol. weight [g/mol]: 207.06
CAS: 53093-42-8

Physical Properties

Property code	Value	Unit	Source
gf	-182.70	kJ/mol	Joback Method
hf	-366.14	kJ/mol	Joback Method
hfus	16.96	kJ/mol	Joback Method
hvap	46.72	kJ/mol	Joback Method
ie	10.07 ± 0.02	eV	NIST Webbook
log10ws	-2.17		Crippen Method
logp	1.865		Crippen Method
mcvol	123.570	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	512.62	K	Joback Method
tc	735.30	K	Joback Method
tf	307.27	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.46	J/mol×K	512.62	Joback Method
cpg	276.29	J/mol×K	549.73	Joback Method
cpg	289.34	J/mol×K	586.85	Joback Method
cpg	301.63	J/mol×K	623.96	Joback Method
cpg	313.18	J/mol×K	661.07	Joback Method
cpg	324.00	J/mol×K	698.19	Joback Method
cpg	334.10	J/mol×K	735.30	Joback Method
dvisc	0.0023129	Pa×s	307.27	Joback Method

dvisc	0.0015206	Pa×s	341.50	Joback Method
dvisc	0.0010791	Pa×s	375.72	Joback Method
dvisc	0.0008109	Pa×s	409.94	Joback Method
dvisc	0.0006368	Pa×s	444.17	Joback Method
dvisc	0.0005177	Pa×s	478.39	Joback Method
dvisc	0.0004326	Pa×s	512.62	Joback Method

Sources

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=C53093428&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume