Acetic acid, bromo-, propyl ester

Other names: Propyl bromoacetate
Inchi: InChI=1S/C5H9BrO2/c1-2-3-8-5(7)4-6/h2-4H2,1H3
InchiKey: ISYUCUGTDNJIHV-UHFFFAOYSA-N
Formula: C5H9BrO2
SMILES: CCCOC(=O)CBr
Mol. weight [g/mol]: 181.03
CAS: 35223-80-4

Physical Properties

Property code	Value	Unit	Source
gf	-228.38	kJ/mol	Joback Method
hf	-365.00	kJ/mol	Joback Method
hfus	16.78	kJ/mol	Joback Method
hvap	42.31	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.334		Crippen Method
mcvol	106.250	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	456.25	K	Joback Method
tc	652.96	K	Joback Method
tf	278.07	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.91	J/mol×K	456.25	Joback Method
cpg	234.86	J/mol×K	620.17	Joback Method
cpg	227.76	J/mol×K	587.39	Joback Method
cpg	220.31	J/mol×K	554.60	Joback Method
cpg	212.52	J/mol×K	521.82	Joback Method
cpg	204.39	J/mol×K	489.03	Joback Method
cpg	241.64	J/mol×K	652.96	Joback Method
dvisc	0.0003528	Pa×s	456.25	Joback Method

dvisc	0.0004391	Pa×s	426.55	Joback Method
dvisc	0.0005647	Pa×s	396.86	Joback Method
dvisc	0.0007565	Pa×s	367.16	Joback Method
dvisc	0.0010668	Pa×s	337.46	Joback Method
dvisc	0.0016076	Pa×s	307.77	Joback Method
dvisc	0.0026445	Pa×s	278.07	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=C35223804&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
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