Bromoacetic acid, pentyl ester

Other names:	Acetic acid, bromo, pentyl ester
	Pentyl bromoacetate
Inchi:	InChI=1S/C7H13BrO2/c1-2-3-4-5-10-7(9)6-8/h2-6H2,1H3
InchiKey:	YOCUEALKMOVVAJ-UHFFFAOYSA-N
Formula:	C7H13BrO2
SMILES:	CCCCCOC(=O)CBr
Mol. weight [g/mol]:	209.08
CAS:	52034-03-4

Physical Properties

Property code	Value	Unit	Source
gf	-211.54	kJ/mol	Joback Method
hf	-406.28	kJ/mol	Joback Method
hfus	21.96	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
logp	2.115		Crippen Method
mcvol	134.430	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
rinpol	1166.70		NIST Webbook
tb	502.01	K	Joback Method
tc	694.06	K	Joback Method
tf	300.61	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.81	J/mol×K	502.01	Joback Method
cpg	326.65	J/mol×K	662.05	Joback Method
cpg	317.59	J/mol×K	630.04	Joback Method
cpg	308.09	J/mol×K	598.04	Joback Method
cpg	298.13	J/mol×K	566.03	Joback Method
cpg	287.70	J/mol×K	534.02	Joback Method

cpg	335.26	J/mol×K	694.06	Joback Method
dvisc	0.0002990	Pa×s	502.01	Joback Method
dvisc	0.0003769	Pa×s	468.44	Joback Method
dvisc	0.0004925	Pa×s	434.88	Joback Method
dvisc	0.0006729	Pa×s	401.31	Joback Method
dvisc	0.0009732	Pa×s	367.74	Joback Method
dvisc	0.0015160	Pa×s	334.18	Joback Method
dvisc	0.0026071	Pa×s	300.61	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52034034&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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