Bromoacetic acid, 2-pentyl ester

Other names: Acetic acid, bromo, 1-methylbutyl ester
Inchi: InChI=1S/C7H13BrO2/c1-3-4-6(2)10-7(9)5-8/h6H,3-5H2,1-2H3
InchiKey: UFZOVZFMSBMLBZ-UHFFFAOYSA-N
Formula: C7H13BrO2
SMILES: CCCC(C)OC(=O)CBr
Mol. weight [g/mol]: 209.08
CAS: 73448-66-5

Physical Properties

Property code	Value	Unit	Source
gf	-213.98	kJ/mol	Joback Method
hf	-411.56	kJ/mol	Joback Method
hfus	18.43	kJ/mol	Joback Method
hvap	46.38	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.113		Crippen Method
mcvol	134.430	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
rinpol	1094.00		NIST Webbook
rinpol	1094.00		NIST Webbook
ripol	1538.00		NIST Webbook
ripol	1538.00		NIST Webbook
tb	501.57	K	Joback Method
tc	697.81	K	Joback Method
tf	285.61	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.07	J/mol×K	501.57	Joback Method
cpg	288.28	J/mol×K	534.28	Joback Method
cpg	298.99	J/mol×K	566.98	Joback Method
cpg	309.20	J/mol×K	599.69	Joback Method

cpg	318.93	J/mol×K	632.40	Joback Method
cpg	328.18	J/mol×K	665.11	Joback Method
cpg	336.97	J/mol×K	697.81	Joback Method
dvisc	0.0034561	Pa×s	285.61	Joback Method
dvisc	0.0018031	Pa×s	321.60	Joback Method
dvisc	0.0010723	Pa×s	357.60	Joback Method
dvisc	0.0007013	Pa×s	393.59	Joback Method
dvisc	0.0004925	Pa×s	429.58	Joback Method
dvisc	0.0003653	Pa×s	465.58	Joback Method
dvisc	0.0002828	Pa×s	501.57	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=C73448665&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume