Bromoacetic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C9H9BrO3/c1-12-7-2-4-8(5-3-7)13-9(11)6-10/h2-5H,6H2,1H3
InchiKey: CWPDVNAECGVQQI-UHFFFAOYSA-N
Formula: C9H9BrO3
SMILES: COc1ccc(OC(=O)CBr)cc1
Mol. weight [g/mol]: 245.07

Physical Properties

Property code	Value	Unit	Source
gf	-196.92	kJ/mol	Joback Method
hf	-354.72	kJ/mol	Joback Method
hfus	21.98	kJ/mol	Joback Method
hvap	56.57	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.995		Crippen Method
mcvol	144.720	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	1575.00		NIST Webbook
rinpol	1575.00		NIST Webbook
tb	601.85	K	Joback Method
tc	830.28	K	Joback Method
tf	384.32	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.49	J/mol×K	601.85	Joback Method
cpg	324.70	J/mol×K	639.92	Joback Method
cpg	335.22	J/mol×K	677.99	Joback Method
cpg	345.05	J/mol×K	716.06	Joback Method
cpg	354.20	J/mol×K	754.14	Joback Method
cpg	362.68	J/mol×K	792.21	Joback Method
cpg	370.48	J/mol×K	830.28	Joback Method
dvisc	0.0011373	Pa×s	384.32	Joback Method

dvisc	0.0007401	Pa×s	420.57	Joback Method
dvisc	0.0005156	Pa×s	456.83	Joback Method
dvisc	0.0003789	Pa×s	493.09	Joback Method
dvisc	0.0002904	Pa×s	529.34	Joback Method
dvisc	0.0002303	Pa×s	565.60	Joback Method
dvisc	0.0001878	Pa×s	601.85	Joback Method

Sources

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=U308048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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