Benzeneacetic acid, «alpha»-bromo-, methyl ester

Other names: Methyl «alpha»-bromophenylacetate
Acetic acid, bromophenyl-, methyl ester
Methyl «alpha»-bromo-«alpha»-phenylacetate
Methyl «alpha»-bromobenzeneacetate
Methyl bromophenylacetate
2-bromo-2-phenylacetic acid methyl ester

Inchi: InChI=1S/C9H9BrO2/c1-12-9(11)8(10)7-5-3-2-4-6-7/h2-6,8H,1H3

InchiKey: NHFBYYMNJUMVOT-UHFFFAOYSA-N

Formula: C9H9BrO2

SMILES: COC(=O)C(Br)c1ccccc1

Mol. weight [g/mol]: 229.07

CAS: 3042-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-84.73	kJ/mol	Joback Method
hf	-216.31	kJ/mol	Joback Method
hfus	17.66	kJ/mol	Joback Method
hvap	53.11	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.296		Crippen Method
mcvol	138.850	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	574.01	K	Joback Method
tc	809.80	K	Joback Method
tf	334.57	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.46	J/mol×K	574.01	Joback Method
cpg	304.43	J/mol×K	613.31	Joback Method
cpg	315.55	J/mol×K	652.61	Joback Method

cpg	325.86	J/mol×K	691.91	Joback Method
cpg	335.38	J/mol×K	731.20	Joback Method
cpg	344.16	J/mol×K	770.50	Joback Method
cpg	352.23	J/mol×K	809.80	Joback Method
dvisc	0.0023666	Pa×s	334.57	Joback Method
dvisc	0.0012995	Pa×s	374.48	Joback Method
dvisc	0.0008009	Pa×s	414.38	Joback Method
dvisc	0.0005374	Pa×s	454.29	Joback Method
dvisc	0.0003846	Pa×s	494.20	Joback Method
dvisc	0.0002893	Pa×s	534.10	Joback Method
dvisc	0.0002265	Pa×s	574.01	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.50 ± 0.50	K	3.30	NIST Webbook

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=C3042817&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume