

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/molxK	574.01	Joback Method
cpg	304.43	J/molxK	613.31	Joback Method
cpg	315.55	J/molxK	652.61	Joback Method

cpg	325.86	J/molxK	691.91	Joback Method
cpg	335.38	J/molxK	731.20	Joback Method
cpg	344.16	J/molxK	770.50	Joback Method
cpg	352.23	J/molxK	809.80	Joback Method
dvisc	0.0023666	Paxs	334.57	Joback Method
dvisc	0.0012995	Paxs	374.48	Joback Method
dvisc	0.0008009	Paxs	414.38	Joback Method
dvisc	0.0005374	Paxs	454.29	Joback Method
dvisc	0.0003846	Paxs	494.20	Joback Method
dvisc	0.0002893	Paxs	534.10	Joback Method
dvisc	0.0002265	Paxs	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3042817&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

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

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