Benzoic acid, 3-bromo-, methyl ester

Other names:	Methyl 3-bromobenzoate
	m-Bromobenzoic acid methyl ester
	Benzoic acid, m-bromo-, methyl ester
	Methyl m-bromobenzoate
	3-Bromobenzoic acid, methyl ester
Inchi:	InChI=1S/C8H7BrO2/c1-11-8(10)6-3-2-4-7(9)5-6/h2-5H,1H3
InchiKey:	KMFJVYMFCAIRAN-UHFFFAOYSA-N
Formula:	C8H7BrO2
SMILES:	COC(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	215.04
CAS:	618-89-3

Physical Properties

Property code	Value	Unit	Source
gf	-100.34	kJ/mol	Joback Method
hf	-201.86	kJ/mol	Joback Method
hfus	18.20	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.236		Crippen Method
mcvol	124.760	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
rinpol	1340.00		NIST Webbook
rinpol	1340.00		NIST Webbook
tb	556.55	K	Joback Method
tc	792.86	K	Joback Method
tf	304.50 ± 0.50	K	NIST Webbook
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.83	J/mol×K	556.55	Joback Method
cpg	257.12	J/mol×K	595.93	Joback Method

cpg	266.74	J/mol×K	635.32	Joback Method
cpg	275.70	J/mol×K	674.70	Joback Method
cpg	284.02	J/mol×K	714.09	Joback Method
cpg	291.72	J/mol×K	753.47	Joback Method
cpg	298.81	J/mol×K	792.86	Joback Method
dvisc	0.0015564	Pa×s	350.82	Joback Method
dvisc	0.0010113	Pa×s	385.11	Joback Method
dvisc	0.0007051	Pa×s	419.40	Joback Method
dvisc	0.0005191	Pa×s	453.69	Joback Method
dvisc	0.0003990	Pa×s	487.97	Joback Method
dvisc	0.0003175	Pa×s	522.26	Joback Method
dvisc	0.0002598	Pa×s	556.55	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.70	K	2.00	NIST Webbook
tbrp	395.60	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C618893&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume