4-Bromo-1,2-(methylenedioxy)benzene

Other names:	3,4-Methylenedioxybromobenzene
	4-Bromomethylenedioxybenzene
	5-bromobenzo-1,3-dioxole
Inchi:	InChI=1S/C7H5BrO2/c8-5-1-2-6-7(3-5)10-4-9-6/h1-3H,4H2
InchiKey:	FBOYMIDCHINJKC-UHFFFAOYSA-N
Formula:	C7H5BrO2
SMILES:	Brc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	201.02
CAS:	2635-13-4

Physical Properties

Property code	Value	Unit	Source
gf	11.75	kJ/mol	Joback Method
hf	-118.75	kJ/mol	Joback Method
hfus	25.46	kJ/mol	Joback Method
hvap	50.45	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.178		Crippen Method
mcvol	104.110	ml/mol	McGowan Method
pc	5289.26	kPa	Joback Method
tb	527.67	K	Joback Method
tc	777.88	K	Joback Method
tf	355.23	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.53	J/mol×K	527.67	Joback Method
cpg	214.91	J/mol×K	569.37	Joback Method
cpg	223.43	J/mol×K	611.07	Joback Method
cpg	231.19	J/mol×K	652.77	Joback Method
cpg	238.26	J/mol×K	694.47	Joback Method
cpg	244.73	J/mol×K	736.17	Joback Method

cpg	250.68	J/mol×K	777.88	Joback Method
dvisc	0.0021301	Pa×s	355.23	Joback Method
dvisc	0.0015957	Pa×s	383.97	Joback Method
dvisc	0.0012444	Pa×s	412.71	Joback Method
dvisc	0.0010024	Pa×s	441.45	Joback Method
dvisc	0.0008291	Pa×s	470.19	Joback Method
dvisc	0.0007010	Pa×s	498.93	Joback Method
dvisc	0.0006035	Pa×s	527.67	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	358.70	K	0.10	NIST Webbook
tbrp	392.50 ± 0.50	K	2.70	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=C2635134&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