1,3-Dioxolane, 2-(3-bromophenyl)-

Other names:	m-Bromobenzaldehyde ethylene acetal
	3-Bromobenzaldehyde ethylene acetal
	2-(3-Bromophenyl)dioxolane
	1,3-Dioxolane, 2-(m-bromophenyl)-
	2-(m-bromophenyl)-1,3-dioxolane
Inchi:	InChI=1S/C9H9BrO2/c10-8-3-1-2-7(6-8)9-11-4-5-12-9/h1-3,6,9H,4-5H2
InchiKey:	VYPYKCPWNPPBBX-UHFFFAOYSA-N
Formula:	C9H9BrO2
SMILES:	Brc1cccc(C2OCCO2)c1
Mol. weight [g/mol]:	229.07
CAS:	17789-14-9

Physical Properties

Property code	Value	Unit	Source
gf	6.31	kJ/mol	Joback Method
hf	-181.22	kJ/mol	Joback Method
hfus	27.90	kJ/mol	Joback Method
hvap	54.28	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.494		Crippen Method
mcvol	132.290	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
tb	572.32	K	Joback Method
tc	829.36	K	Joback Method
tf	353.97	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.33	J/mol×K	572.32	Joback Method
cpg	309.57	J/mol×K	615.16	Joback Method
cpg	322.63	J/mol×K	658.00	Joback Method
cpg	334.59	J/mol×K	700.84	Joback Method

cpg	345.53	J/mol×K	743.68	Joback Method
cpg	355.50	J/mol×K	786.52	Joback Method
cpg	364.60	J/mol×K	829.36	Joback Method
dvisc	0.0025148	Pa×s	353.97	Joback Method
dvisc	0.0015697	Pa×s	390.36	Joback Method
dvisc	0.0010618	Pa×s	426.75	Joback Method
dvisc	0.0007638	Pa×s	463.14	Joback Method
dvisc	0.0005764	Pa×s	499.54	Joback Method
dvisc	0.0004519	Pa×s	535.93	Joback Method
dvisc	0.0003655	Pa×s	572.32	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	405.70	K	1.00	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=C17789149&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