1-BROMO-2,4-DIMETHOXYBENZENE

Other names:	1-Bromo-2,4-dimethoxybenzene
	4-Bromo-1,3-dimethoxybenzene
	4-Bromoresorcinol dimethyl ether
	2,4-Dimethoxybromobenzene
	2,4-Dimethoxyphenyl bromide
Inchi:	InChI=1S/C8H9BrO2/c1-10-6-3-4-7(9)8(5-6)11-2/h3-5H,1-2H3
InchiKey:	NIUZVSQOXJIHBL-UHFFFAOYSA-N
Formula:	C8H9BrO2
SMILES:	COc1ccc(Br)c(OC)c1
Mol. weight [g/mol]:	217.06

Physical Properties

Property code	Value	Unit	Source
hf	-200.34	kJ/mol	Cheméo Relay (1.0)
hfus	17.40	kJ/mol	Joback Method
hvap	70.26	kJ/mol	Cheméo Relay (1.0)
ie	7.97	eV	Cheméo Relay (1.0)
log10ws	-3.33		Cheméo Relay (1.0)
logp	2.466		Crippen Method
mcvol	129.060	ml/mol	McGowan Method
tb	527.44	K	Cheméo Relay (1.0)
tf	311.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.01	J/mol×K	530.08	Joback Method
cpg	266.93	J/mol×K	567.71	Joback Method
cpg	277.32	J/mol×K	605.35	Joback Method
cpg	287.19	J/mol×K	642.98	Joback Method
cpg	296.52	J/mol×K	680.61	Joback Method
cpg	305.31	J/mol×K	718.25	Joback Method
cpg	313.56	J/mol×K	755.88	Joback Method
dvisc	0.0010073	Pa×s	335.64	Joback Method

dvisc	0.0006754	Pa×s	368.05	Joback Method
dvisc	0.0004832	Pa×s	400.45	Joback Method
dvisc	0.0003634	Pa×s	432.86	Joback Method
dvisc	0.0002844	Pa×s	465.27	Joback Method
dvisc	0.0002298	Pa×s	497.67	Joback Method
dvisc	0.0001906	Pa×s	530.08	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	427.20	K	2.40	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17715694&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tf: Normal melting (fusion) point