Benzene, 1-(2-bromoethyl)-4-methoxy-

Other names:	Anisole, p-(2-bromoethyl)-
	p-(2-Bromoethyl)anisole
	p-Methoxyphenethyl bromide
	p-Methoxyphenylethyl bromide
	4-Methoxyphenethyl bromide
	1-(2-Bromoethyl)-4-methoxybenzene
	1-Bromo-2-(4-methoxyphenyl)ethane
Inchi:	InChI=1S/C9H11BrO/c1-11-9-4-2-8(3-5-9)6-7-10/h2-5H,6-7H2,1H3
InchiKey:	OXHPTABOQVHKLN-UHFFFAOYSA-N
Formula:	C9H11BrO
SMILES:	COc1ccc(CCBr)cc1
Mol. weight [g/mol]:	215.09
CAS:	14425-64-0

Physical Properties

Property code	Value	Unit	Source
gf	37.00	kJ/mol	Joback Method
hf	-109.92	kJ/mol	Joback Method
hfus	19.19	kJ/mol	Joback Method
hvap	47.41	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
log10ws	-2.83		Crippen Method
logp	2.633		Crippen Method
mcvol	137.280	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
tb	525.56	K	Joback Method
tc	748.86	K	Joback Method
tf	312.16	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.46	J/mol×K	525.56	Joback Method

cpg	290.03	J/mol×K	562.78	Joback Method
cpg	301.88	J/mol×K	599.99	Joback Method
cpg	313.03	J/mol×K	637.21	Joback Method
cpg	323.50	J/mol×K	674.42	Joback Method
cpg	333.31	J/mol×K	711.64	Joback Method
cpg	342.49	J/mol×K	748.86	Joback Method
dvisc	0.0016608	Pa×s	312.16	Joback Method
dvisc	0.0010004	Pa×s	347.73	Joback Method
dvisc	0.0006621	Pa×s	383.29	Joback Method
dvisc	0.0004700	Pa×s	418.86	Joback Method
dvisc	0.0003520	Pa×s	454.43	Joback Method
dvisc	0.0002749	Pa×s	489.99	Joback Method
dvisc	0.0002221	Pa×s	525.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14425640&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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume