4-Bromo-3-nitroanisole

Other names:	4-Bromo-3-nitroanisol
	Benzene, 1-bromo-4-methoxy-2-nitro-
Inchi:	InChI=1S/C7H6BrNO3/c1-12-5-2-3-6(8)7(4-5)9(10)11/h2-4H,1H3
InchiKey:	KCOBIBRGPCFIGF-UHFFFAOYSA-N
Formula:	C7H6BrNO3
SMILES:	COc1ccc(Br)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	232.03
CAS:	5344-78-5

Physical Properties

Property code	Value	Unit	Source
gf	46.08	kJ/mol	Joback Method
hf	-90.87	kJ/mol	Joback Method
hfus	24.98	kJ/mol	Joback Method
hvap	60.21	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.366		Crippen Method
mcvol	126.520	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
tb	636.62	K	Joback Method
tc	896.89	K	Joback Method
tf	445.75	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.92	J/mol×K	636.62	Joback Method
cpg	280.49	J/mol×K	680.00	Joback Method
cpg	289.32	J/mol×K	723.38	Joback Method
cpg	297.43	J/mol×K	766.75	Joback Method
cpg	304.84	J/mol×K	810.13	Joback Method
cpg	311.58	J/mol×K	853.51	Joback Method
cpg	317.66	J/mol×K	896.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5344785&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume