4-Bromo-3-nitrotoluene

Other names: Benzene, 1-bromo-4-methyl-2-nitro-
Inchi: InChI=1S/C7H6BrNO2/c1-5-2-3-6(8)7(4-5)9(10)11/h2-4H,1H3
InchiKey: UPBUTKQMDPHQAQ-UHFFFAOYSA-N
Formula: C7H6BrNO2
SMILES: Cc1ccc(Br)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 216.03
CAS: 5326-34-1

Physical Properties

Property code	Value	Unit	Source
gf	151.08	kJ/mol	Joback Method
hf	41.35	kJ/mol	Joback Method
hfus	23.79	kJ/mol	Joback Method
hvap	57.80	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.666		Crippen Method
mcvol	120.650	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
tb	614.20	K	Joback Method
tc	879.26	K	Joback Method
tf	423.52	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.82	J/mol×K	614.20	Joback Method
cpg	259.45	J/mol×K	658.38	Joback Method
cpg	268.29	J/mol×K	702.55	Joback Method
cpg	276.39	J/mol×K	746.73	Joback Method
cpg	283.80	J/mol×K	790.91	Joback Method
cpg	290.58	J/mol×K	835.09	Joback Method
cpg	296.77	J/mol×K	879.26	Joback Method

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=C5326341&Units=SI

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