2-Bromo-4-methyl-6-nitrophenol

Inchi: InChI=1S/C7H6BrNO3/c1-4-2-5(8)7(10)6(3-4)9(11)12/h2-3,10H,1H3
InchiKey: ABMPSIRCVCUHLO-UHFFFAOYSA-N
Formula: C7H6BrNO3
SMILES: Cc1cc(Br)c(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 232.03
CAS: 20039-91-2

Physical Properties

Property code	Value	Unit	Source
gf	-3.54	kJ/mol	Joback Method
hf	-135.96	kJ/mol	Joback Method
hfus	29.58	kJ/mol	Joback Method
hvap	70.82	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.371		Crippen Method
mcvol	126.520	ml/mol	McGowan Method
pc	5414.53	kPa	Joback Method
tb	694.82	K	Joback Method
tc	967.26	K	Joback Method
tf	535.24	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.18	J/mol×K	694.82	Joback Method
cpg	294.28	J/mol×K	740.23	Joback Method
cpg	301.80	J/mol×K	785.63	Joback Method
cpg	308.88	J/mol×K	831.04	Joback Method
cpg	315.66	J/mol×K	876.45	Joback Method
cpg	322.26	J/mol×K	921.86	Joback Method
cpg	328.81	J/mol×K	967.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20039912&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
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