4-bromo-3-nitrobenzoic acid

Inchi: InChI=1S/C7H4BrNO4/c8-5-2-1-4(7(10)11)3-6(5)9(12)13/h1-3H,(H,10,11)
InchiKey: RVCTZJVBWNFYRU-UHFFFAOYSA-N
Formula: C7H4BrNO4
SMILES: O=C(O)c1ccc(Br)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 246.02

Physical Properties

Property code	Value	Unit	Source
gf	-114.66	kJ/mol	Joback Method
hf	-223.46	kJ/mol	Joback Method
hfus	29.48	kJ/mol	Joback Method
hvap	81.23	kJ/mol	Joback Method
log10ws	-2.97		Aqueous Solubility Prediction Method
logp	2.055		Crippen Method
mcvol	128.090	ml/mol	McGowan Method
pc	5462.66	kPa	Joback Method
tb	760.25	K	Joback Method
tc	1005.17	K	Joback Method
tf	476.65	K	Aqueous Solubility Prediction Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.50	J/mol×K	760.25	Joback Method
cpg	295.74	J/mol×K	801.07	Joback Method
cpg	301.41	J/mol×K	841.89	Joback Method
cpg	306.57	J/mol×K	882.71	Joback Method
cpg	311.24	J/mol×K	923.53	Joback Method
cpg	315.48	J/mol×K	964.35	Joback Method
cpg	319.32	J/mol×K	1005.17	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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