Benzamide, N-(3-nitrophenyl)-2-bromo-

Inchi: InChI=1S/C13H9BrN2O3/c14-12-7-2-1-6-11(12)13(17)15-9-4-3-5-10(8-9)16(18)19/h1-8H
InchiKey: SMAIGFKAVOUSHO-UHFFFAOYSA-N
Formula: C13H9BrN2O3
SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)c1ccccc1Br
Mol. weight [g/mol]: 321.13

Physical Properties

Property code	Value	Unit	Source
gf	274.48	kJ/mol	Joback Method
hf	94.93	kJ/mol	Joback Method
hfus	40.07	kJ/mol	Joback Method
hvap	86.62	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	3.610		Crippen Method
mcvol	192.980	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	2604.00		NIST Webbook
rinpol	2604.00		NIST Webbook
tb	882.20	K	Joback Method
tc	1158.52	K	Joback Method
tf	620.15	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.66	J/mol×K	882.20	Joback Method
cpg	515.19	J/mol×K	928.25	Joback Method
cpg	523.72	J/mol×K	974.31	Joback Method
cpg	531.37	J/mol×K	1020.36	Joback Method
cpg	538.27	J/mol×K	1066.41	Joback Method
cpg	544.52	J/mol×K	1112.47	Joback Method
cpg	550.25	J/mol×K	1158.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307390&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume