Benzamide, 2-bromo-N-(4-bromophenyl)-

Other names: Benzamide, N-(4-bromophenyl)-2-bromo-
Inchi: InChI=1S/C13H9Br2NO/c14-9-5-7-10(8-6-9)16-13(17)11-3-1-2-4-12(11)15/h1-8H,(H,16,1
InchiKey: FYSAKWBWAQDJDE-UHFFFAOYSA-N
Formula: C13H9Br2NO
SMILES: O=C(Nc1ccc(Br)cc1)c1ccccc1Br
Mol. weight [g/mol]: 355.02
CAS: 66569-07-1

Physical Properties

Property code	Value	Unit	Source
gf	253.25	kJ/mol	Joback Method
hf	132.02	kJ/mol	Joback Method
hfus	34.00	kJ/mol	Joback Method
hvap	76.46	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.464		Crippen Method
mcvol	193.060	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
rinpol	2464.00		NIST Webbook
rinpol	2464.00		NIST Webbook
tb	796.52	K	Joback Method
tc	1067.35	K	Joback Method
tf	536.34	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.54	J/mol×K	796.52	Joback Method
cpg	461.07	J/mol×K	841.66	Joback Method
cpg	470.60	J/mol×K	886.80	Joback Method
cpg	479.26	J/mol×K	931.93	Joback Method
cpg	487.17	J/mol×K	977.07	Joback Method
cpg	494.43	J/mol×K	1022.21	Joback Method

cpg	501.19	J/mol×K	1067.35	Joback Method

Sources

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=C66569071&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume