

Benzamide, N-(4-bromophenyl)-3-bromo-

Inchi:	InChI=1S/C13H9Br2NO/c14-10-4-6-12(7-5-10)16-13(17)9-2-1-3-11(15)8-9/h1-8H,(H,16,17)
InchiKey:	RNMIDZORNPWDTP-UHFFFAOYSA-N
Formula:	C13H9Br2NO
SMILES:	O=C(Nc1ccc(Br)cc1)c1cccc(Br)c1
Mol. weight [g/mol]:	355.02

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
rinpola	2559.00		NIST Webbook
rinpola	2559.00		NIST Webbook
tb	796.52	K	Joback Method
tc	1067.35	K	Joback Method
tf	536.34	K	Joback Method
vc	0.713	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.54	J/molxK	796.52	Joback Method
cpg	461.07	J/molxK	841.66	Joback Method
cpg	470.60	J/molxK	886.80	Joback Method
cpg	479.26	J/molxK	931.93	Joback Method
cpg	487.17	J/molxK	977.07	Joback Method
cpg	494.43	J/molxK	1022.21	Joback Method
cpg	501.19	J/molxK	1067.35	Joback Method

Sources

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=U307156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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