

3-Bromobenzoic acid hydrazide

Other names:	3-Bromobenzhydrazide Benzoic acid, 3-bromo-, hydrazide Benzoic acid, m-bromo-, hydrazide (3-Bromobenzoyl)hydrazine (m-Bromobenzoyl)hydrazine m-Bromobenzohydrazide m-Bromobenzoic acid hydrazide m-Bromobenzoic hydrazide
Inchi:	InChI=1S/C7H7BrN2O/c8-6-3-1-2-5(4-6)7(11)10-9/h1-4H,9H2,(H,10,11)
InchiKey:	BNAQRAZIPAHWAR-UHFFFAOYSA-N
Formula:	C7H7BrN2O
SMILES:	<chem>NNC(=O)c1cccc(Br)c1</chem>
Mol. weight [g/mol]:	215.05
CAS:	39115-96-3

Physical Properties

Property code	Value	Unit	Source
gf	152.08	kJ/mol	Joback Method
hf	38.26	kJ/mol	Joback Method
hfus	24.72	kJ/mol	Joback Method
hvap	64.37	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	1.053		Crippen Method
mcvol	124.760	ml/mol	McGowan Method
pc	5312.41	kPa	Joback Method
tb	633.95	K	Joback Method
tc	884.23	K	Joback Method
tf	453.24	K	Joback Method
vc	0.452	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.17	J/molxK	633.95	Joback Method

cpg	280.43	J/mol×K	675.66	Joback Method
cpg	288.92	J/mol×K	717.38	Joback Method
cpg	296.67	J/mol×K	759.09	Joback Method
cpg	303.75	J/mol×K	800.80	Joback Method
cpg	310.21	J/mol×K	842.52	Joback Method
cpg	316.09	J/mol×K	884.23	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=C39115963&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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