

p-Bromobenzoic acid hydrazide

Other names:	p-Bromobenzhydrazide 4-Bromobenzhydrazide p-Bromobenzoic acid hydrazide Benzoic acid, 4-bromo-, hydrazide Benzoic acid, p-bromo-, hydrazide 4-bromobenzohydrazide
Inchi:	InChI=1S/C7H7BrN2O/c8-6-3-1-5(2-4-6)7(11)10-9/h1-4H,9H2,(H,10,11)
InchiKey:	UYIMBYKIIMYFPS-UHFFFAOYSA-N
Formula:	C7H7BrN2O
SMILES:	NNC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]:	215.05

Physical Properties

Property code	Value	Unit	Source
hf	1.86	kJ/mol	Cheméo Relay (1.0)
hfus	24.72	kJ/mol	Joback Method
ie	9.01	eV	Cheméo Relay (1.0)
log10ws	-2.39		Cheméo Relay (1.0)
logp	1.053		Crippen Method
mcvol	124.760	ml/mol	McGowan Method
tb	590.69	K	Cheméo Relay (1.0)
tf	433.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.17	J/mol×K	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

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5933324&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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