Benzamide, 2-bromo-

Other names:	Benzamide, o-bromo- o-Bromobenzamide 2-Bromobenzamide
Inchi:	InChI=1S/C7H6BrNO/c8-6-4-2-1-3-5(6)7(9)10/h1-4H,(H2,9,10)
InchiKey:	NHNAEZDWNCRWRW-UHFFFAOYSA-N
Formula:	C7H6BrNO
SMILES:	NC(=O)c1ccccc1Br
Mol. weight [g/mol]:	200.03
CAS:	4001-73-4

Physical Properties

Property code	Value	Unit	Source
gf	62.69	kJ/mol	Joback Method
hf	-15.21	kJ/mol	Joback Method
hfus	19.62	kJ/mol	Joback Method
hvap	57.94	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	1.548		Crippen Method
mcvol	114.780	ml/mol	McGowan Method
pc	5213.15	kPa	Joback Method
tb	583.78	K	Joback Method
tc	837.04	K	Joback Method
tf	400.58	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.12	J/mol×K	583.78	Joback Method
cpg	239.29	J/mol×K	625.99	Joback Method
cpg	247.70	J/mol×K	668.20	Joback Method
cpg	255.39	J/mol×K	710.41	Joback Method
cpg	262.43	J/mol×K	752.62	Joback Method
cpg	268.85	J/mol×K	794.83	Joback Method

cpg	274.71	J/mol×K	837.04	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=C4001734&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume