M-BROMOACETANILIDE

Other names:	3'-bromoacetanilide
	3-bromoacetanilide
	Acetanilide, 3'-bromo-
	N-(3-Bromophenyl)acetic acid amide
	N-(3-bromophenyl)acetamide
	N-acetyl-3-bromoaniline
	meta-bromoacetanilide
Inchi:	InChI=1S/C8H8BrNO/c1-6(11)10-8-4-2-3-7(9)5-8/h2-5H,1H3,(H,10,11)
InchiKey:	XXHOHJTVFUJJMT-UHFFFAOYSA-N
Formula:	C8H8BrNO
SMILES:	CC(=O)Nc1cccc(Br)c1
Mol. weight [g/mol]:	214.06

Physical Properties

Property code	Value	Unit	Source
hf	-117.38	kJ/mol	Cheméo Relay (1.0)
hfus	22.11	kJ/mol	Joback Method
ie	8.60 ± 0.20	eV	NIST Webbook
log10ws	-2.54		Cheméo Relay (1.0)
logp	2.408		Crippen Method
mcvol	128.870	ml/mol	McGowan Method
tb	559.11	K	Cheméo Relay (1.0)
tf	344.74	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.43	J/mol×K	584.30	Joback Method
cpg	278.04	J/mol×K	624.00	Joback Method
cpg	287.86	J/mol×K	663.70	Joback Method
cpg	296.93	J/mol×K	703.40	Joback Method
cpg	305.29	J/mol×K	743.10	Joback Method
cpg	312.99	J/mol×K	782.80	Joback Method
cpg	320.08	J/mol×K	822.49	Joback Method

Sources

Cheméo Relay (1.0, beta):	
Sublimation enthalpies of 9 substituted acetanilides at 298 K estimated by solution calorimetry approach:	https://www.doi.org/10.1016/j.tca.2017.08.011
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C621385&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