2-Acetamino-5-bromobenzoic acid

Other names:	N-Acetyl-5-bromo-anthranilic acid
	2-Acetamido-5-bromobenzoic acid
	Benzoic acid, 2-(acetylamino)-5-bromo-
	2-Acetylamino-5-bromobenzoic acid
Inchi:	InChI=1S/C9H8BrNO3/c1-5(12)11-8-3-2-6(10)4-7(8)9(13)14/h2-4H,1H3,(H,11,12)(H,13,1
InchiKey:	QVABAFHRLMDDLM-UHFFFAOYSA-N
Formula:	C9H8BrNO3
SMILES:	CC(=O)Nc1ccc(Br)cc1C(=O)O
Mol. weight [g/mol]:	258.07
CAS:	38985-79-4

Physical Properties

Property code	Value	Unit	Source
gf	-172.90	kJ/mol	Joback Method
hf	-313.09	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	82.27	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.106		Crippen Method
mcvol	150.400	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
tb	758.21	K	Joback Method
tc	980.18	K	Joback Method
tf	515.79	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.01	J/mol×K	758.21	Joback Method
cpg	368.75	J/mol×K	795.20	Joback Method
cpg	375.90	J/mol×K	832.20	Joback Method
cpg	382.48	J/mol×K	869.19	Joback Method
cpg	388.53	J/mol×K	906.19	Joback Method

cpg	394.08	J/mol×K	943.18	Joback Method
cpg	399.17	J/mol×K	980.18	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=C38985794&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

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