

2-AMINOACETANILIDE

Other names:	Acetamide, N-(2-aminophenyl)-
Inchi:	InChI=1S/C8H10N2O/c1-6(11)10-8-5-3-2-4-7(8)9/h2-5H,9H2,1H3,(H,10,11)
InchiKey:	MPXAYYWSDIKNTP-UHFFFAOYSA-N
Formula:	C8H10N2O
SMILES:	CC(=O)Nc1ccccc1N
Mol. weight [g/mol]:	150.18

Physical Properties

Property code	Value	Unit	Source
hf	-127.30	kJ/mol	Cheméo Relay (1.0)
hfus	22.02	kJ/mol	Joback Method
ie	7.39 ± 0.02	eV	NIST Webbook
log10ws	-1.15		Cheméo Relay (1.0)
logp	1.227		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
tb	566.81	K	Cheméo Relay (1.0)
tf	383.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.50	J/mol×K	590.67	Joback Method
cpg	297.98	J/mol×K	629.44	Joback Method
cpg	308.67	J/mol×K	668.21	Joback Method
cpg	318.60	J/mol×K	706.98	Joback Method
cpg	327.79	J/mol×K	745.75	Joback Method
cpg	336.28	J/mol×K	784.52	Joback Method
cpg	344.12	J/mol×K	823.28	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34801097&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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