

(2E)-3-(2-aminophenyl)-2-propenoic acid

Inchi:	InChI=1S/C9H9NO2/c10-8-4-2-1-3-7(8)5-6-9(11)12/h1-6H,10H2,(H,11,12)/b6-5+
InchiKey:	KMBQKHKEEHEPOE-AATRIKPKSA-N
Formula:	C9H9NO2
SMILES:	<chem>Nc1cccc1C=CC(=O)O</chem>
Mol. weight [g/mol]:	163.17

Physical Properties

Property code	Value	Unit	Source
gf	8.61	kJ/mol	Joback Method
hf	-117.83	kJ/mol	Joback Method
hfus	23.80	kJ/mol	Joback Method
hvap	72.59	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	1.367		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	4432.62	kPa	Joback Method
tb	659.72	K	Joback Method
tc	879.89	K	Joback Method
tf	419.06	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.42	J/molxK	659.72	Joback Method
cpg	319.65	J/molxK	696.41	Joback Method
cpg	328.23	J/molxK	733.11	Joback Method
cpg	336.20	J/molxK	769.80	Joback Method
cpg	343.60	J/molxK	806.50	Joback Method
cpg	350.48	J/molxK	843.19	Joback Method
cpg	356.90	J/molxK	879.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=B6001565&Units=SI

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
mccvol:	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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