

# naepaine

**Inchi:** InChI=1S/C14H22N2O2/c1-2-3-4-9-16-10-11-18-14(17)12-5-7-13(15)8-6-12/h5-8,16H,2-  
**InchiKey:** UYXHCVFxDBNRQW-UHFFFAOYSA-N  
**Formula:** C14H22N2O2  
**SMILES:** CCCCCNCCOC(=O)c1ccc(N)cc1  
**Mol. weight [g/mol]:** 250.34

## Physical Properties

Property code	Value	Unit	Source
gf	91.70	kJ/mol	Joback Method
hf	-264.77	kJ/mol	Joback Method
hfus	38.75	kJ/mol	Joback Method
hvap	75.93	kJ/mol	Joback Method
log10ws	-3.27		Aqueous Solubility Prediction Method
logp	2.205		Crippen Method
mvol	211.760	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
tb	750.37	K	Joback Method
tc	958.84	K	Joback Method
tf	494.56	K	Joback Method
vc	0.799	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.90	J/mol×K	750.37	Joback Method
cpg	629.61	J/mol×K	785.11	Joback Method
cpg	643.36	J/mol×K	819.86	Joback Method
cpg	656.19	J/mol×K	854.60	Joback Method
cpg	668.11	J/mol×K	889.35	Joback Method
cpg	679.16	J/mol×K	924.09	Joback Method
cpg	689.37	J/mol×K	958.84	Joback Method

# Sources

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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