

Phenylpropanamide

Other names:	3-Phenylpropionamide «beta»-Phenylpropionamide Benzenepropanamide Hydrocinnamamide 3-Phenylpropanamide Amide hydrocinnamique
Inchi:	InChI=1S/C9H11NO/c10-9(11)7-6-8-4-2-1-3-5-8/h1-5H,6-7H2,(H2,10,11)
InchiKey:	VYIBCOSBNVFEIW-UHFFFAOYSA-N
Formula:	C9H11NO
SMILES:	N=C(O)CCc1ccccc1
Mol. weight [g/mol]:	149.19
CAS:	102-93-2

Physical Properties

Property code	Value	Unit	Source
gf	204.09	kJ/mol	Joback Method
hf	53.54	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.154		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
rinpol	1528.40		NIST Webbook
rinpol	1528.40		NIST Webbook
tb	608.52	K	Joback Method
tf	347.21	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.83	J/mol×K	608.52	Joback Method
cpg	30.63	J/mol×K	100.12	Joback Method
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C102932&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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