2-Propenamide, 3-phenyl-

Other names:	Cinnamamide
	2-Benzylideneacetamide
	3-Phenylacrylamide
	3-Phenylpropenamide
	Cinnamide
	Cinnamic amide
	Benzylidene acetamide
	3-Phenyl-2-propenamide
Inchi:	InChI=1S/C9H9NO/c10-9(11)7-6-8-4-2-1-3-5-8/h1-7H,(H2,10,11)/b7-6+
InchiKey:	APEJMQOBVMLION-VOTSOKGWSA-N
Formula:	C9H9NO
SMILES:	NC(=O)C=Cc1ccccc1
Mol. weight [g/mol]:	147.17
CAS:	621-79-4

Physical Properties

Property code	Value	Unit	Source
chs	-4720.60	kJ/mol	NIST Webbook
gf	155.06	kJ/mol	Joback Method
hf	45.87	kJ/mol	Joback Method
hfs	-106.90	kJ/mol	NIST Webbook
hfus	20.11	kJ/mol	Joback Method
hvap	55.25	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.185		Crippen Method
mcvol	121.160	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
tb	562.56	K	Joback Method
tc	801.58	K	Joback Method
tf	345.72	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.31	J/mol×K	562.56	Joback Method
cpg	280.35	J/mol×K	602.40	Joback Method
cpg	291.45	J/mol×K	642.23	Joback Method
cpg	301.67	J/mol×K	682.07	Joback Method
cpg	311.08	J/mol×K	721.90	Joback Method
cpg	319.74	J/mol×K	761.74	Joback Method
cpg	327.72	J/mol×K	801.58	Joback Method

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=C621794&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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