Phenylpropiolamide

Other names: 3-Phenylpropynoic acid amide
Inchi: InChI=1S/C9H7NO/c10-9(11)7-6-8-4-2-1-3-5-8/h1-5H,(H2,10,11)
InchiKey: HJZZEVFDPBDIDQ-UHFFFAOYSA-N
Formula: C9H7NO
SMILES: NC(=O)C#Cc1ccccc1
Mol. weight [g/mol]: 145.16
CAS: 7223-30-5

Physical Properties

Property code	Value	Unit	Source
chs	-4589.40	kJ/mol	NIST Webbook
gf	277.64	kJ/mol	Joback Method
hf	200.95	kJ/mol	Joback Method
hfl	47.40 ± 4.00	kJ/mol	NIST Webbook
hfs	-20.00	kJ/mol	NIST Webbook
hfus	23.03	kJ/mol	Joback Method
hvap	57.44	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	0.523		Crippen Method
mcvol	116.860	ml/mol	McGowan Method
pc	4621.41	kPa	Joback Method
tb	567.40	K	Joback Method
tc	826.44	K	Joback Method
tf	456.90	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.36	J/mol×K	567.40	Joback Method
cpg	260.79	J/mol×K	610.57	Joback Method
cpg	271.30	J/mol×K	653.75	Joback Method
cpg	280.97	J/mol×K	696.92	Joback Method
cpg	289.83	J/mol×K	740.09	Joback Method

cpg	297.94	J/mol×K	783.27	Joback Method
cpg	305.34	J/mol×K	826.44	Joback Method

Sources

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=C7223305&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfl:	Liquid phase 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